Derivation of planar three-body hyperspherical harmonics from monopole harmonics

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(Received 16 September 1996; revised manuscript received 23 January 1997)

The hyperspherical harmonics which appear in the analysis of the planar three-body problem are explicitly expressed in terms of the harmonics of importance in the theory of magnetic monopoles. This connection is achieved by transforming the eigenvalue equations which define hyperspherical harmonics into the eigenvalue equations for monopole harmonics. This transformation requires the recognition of a gauge potential which arises in the three-body problem and which has the same form as that of a magnetic monopole. In this manner, explicit formulas for the two standard representations of the three-body harmonics are derived. The coupling coefficients between the two representations follow naturally from the derivation. Emphasis is placed on the gauge theoretical aspects of the derivations and the significance of gauge transformations is discussed. [S1050-2947(97)10006-3]

PACS number(s): 03.65.Ca, 02.40.−k, 02.20.−a

I. INTRODUCTION

Hyperspherical methods have long been a valuable analytical and computational tool for understanding n-body quantum systems. The original work in this field dates back to at least the time of Fock's treatment of the helium atom [1]. Since then, a large literature has arisen, applying numerous hyperspherical methods (including the hyperspherical harmonics of interest in this article) to the diverse fields of molecular, nuclear, and atomic physics [2–8]. In molecular physics, for example, the hyperspherical approach has played a central role over the last 20 years in the study of reactive scattering. The initial foundation for these studies can be traced to Kuppermann's paper [9] outlining the application of symmetrical hyperspherical coordinates to reactive scattering. Since the original studies on the $H_2+H\rightarrow H+H_2$ reaction, the hyperspherical approach has been successful in treating a number of reactions with increasing computational sophistication [10–16]. In addition, to reactive scattering, hyperspherical techniques have been applied to problems in collision induced dissociation [17] and photodissociation [18], as well as bound-state problems [19,20]. As an example of the latter, Aquilanti *et al.* have analyzed H_2^+ with the aid of Sturmian bases [21]. This method is intimately tied to the momentum space approach of constructing hydrogenlike orbitals through the use of hyperspherical harmonics [7,22]. The hyperspherical approach, in particular, the use of hyperspherical harmonics, has also been extensively applied to nuclear physics, such as in the study of three nucleon systems [5] and recently in studies of halo nuclei consisting of a core surrounded by two loosely bound neutrons [6,23]. In atomic physics hyperspherical techniques have offered significant insight into the doubly excited states of helium [8]. In addition, hyperspherical harmonics have played a central role in the study by Cavagnero on electron correlations in atoms [24–26]. It may also be added that the general nature of hyperspherical techniques makes them particularly useful for investigations which seek to treat diverse phenomena in a coherent fashion and in so doing unify approaches from different fields.

The underlying idea behind all hyperspherical approaches is to consider the n-body configuration space as a multidimensional space with the n-body collision at the origin. The radial distance from the origin is called the hyper-radius. The hyper-radius is a recurring quantity in hyperspherical treatments and is central to many applications, in part, due to its nearly separable nature (in an adiabatic sense) in many problems [27,28,8]. In addition to the hyper-radius, it is often useful to introduce a set of hyperangles to form a complete system of coordinates on configuration space.

The metric used in defining the hyper-radius is specially chosen so that the kinetic-energy operator is proportional to the Laplacian. The kinetic energy then splits into a term dependent only on the hyperradius and a second term which contains all of the angular derivatives. It is this splitting which makes useful the introduction of hyperspherical harmonics, defined as eigenfunctions of the angular term of the kinetic energy. These harmonics have been used as basis functions for expansions of the n-body wave functions and potential-energy surfaces.

Smith [29] was one of the first to consider hyperspherical harmonics in the context of the quantum n-body problem. Though Smith's original work focused on the planar three-body problem, the use of hyperspherical harmonics has since been generalized and developed extensively. However, properties of the hyperspherical harmonics are still not completely understood, and efficient mathematical methods for exploiting them in concrete problems remain elusive. For example, there is the question of how to construct the coupling coefficients between different bases of hyperspherical harmonics [2]. This issue is of key importance when one wishes to transform between two different choices of commuting observables, and such transformations have been especially useful in mapping potential-energy surfaces between different choices of hyperangles [30,31,2]. Though the problem of coupling coefficients is not the primary focus of our paper, it is expected that our methods will, nevertheless, shine light on this issue.

Our main result in this paper is an approach for generating the planar three-body hyperspherical harmonics, wherein we express them in terms of monopole harmonics. This connection between Smith's hyperspherical harmonics and monopole harmonics arises from the existence of a gauge potential, first realized by Guichardet [32], in the n-body problem. For the three-body problem, this gauge potential was shown by Iwai [33] to be of the same form as the gauge potential of a magnetic monopole. The gauge potential arises when one separates rotations from internal motions, and it is associated with a choice of body frame. The gauge potential is found naturally in expressions for the angular momentum and kinetic energy when written in terms of shape and orientation coordinates. As we shall show, the gauge potential also arises in expressions for the operators which define the hyperspherical harmonics. These expressions ultimately allow the eigenvalue problem of Smith's to be turned into the eigenvalue problem for magnetic monopoles, whose solutions are the monopole harmonics. Monopole harmonics are well studied. Basic references are Wu and Yang [34] and Biedenharn and Louck [35].

The gauge theoretic methods applied here to the planar three-body problem are part of a larger branch of research concerning gauge fields in the n-body problem, which is reviewed by Littlejohn and Reinsch [36]. The gauge theory of the n-body problem is itself an example of a geometric phase and belongs to the same class of problems as Berry's phase and the geometric phases which arise in the Born-Oppenheimer theory [37] and optics. Much research on geometric phases has been presented in the connection theory of fiber bundles, which is the proper mathematical setting for these problems. All the results presented here, however, will be derived by more conventional techniques.

In Sec. II, we present the relevant background on magnetic monopoles, which is drawn mainly from Ref. [34]. In Sec. III, we define several coordinate systems on the three-body configuration space and introduce conventions for the body frame. In Sec. III C the gauge potential is introduced and discussed. Section IV is the heart of the paper, in which we analyze the group SO(4) and a certain SU(2) subgroup from the gauge theoretical viewpoint. In Sec. IV D, the operators which define the hyperspherical harmonics are expressed in terms of the gauge potential. In Sec. V we present our derivation of the hyperspherical harmonics in the two conventions first introduced by Smith. The coupling coefficients between these two sets of harmonics (also derived by Smith) follow readily from our approach.

II. MAGNETIC MONOPOLES

We present here a brief survey of magnetic monopoles and the associated monopole harmonics [38,34]. The magnetic field of a monopole of magnetic charge g centered at the origin is

$$\mathbf{B}=g\,\frac{\mathbf{x}}{|\mathbf{x}|^3}. \tag{2.1}$$

The gauge potential of this magnetic field is expressed in what we call the "north regular gauge" as

$$\mathbf{A}^{\mathrm{NR}}=g\,\frac{1-\cos\theta}{|\mathbf{x}|\sin\theta}\,\hat{\boldsymbol{\phi}}, \tag{2.2}$$

where θ and ϕ are the usual spherical coordinates. We say that $\mathbf{A}^{\mathrm{NR}}$ is in the north regular gauge because the gauge potential possesses no singularities in the upper half-space $(x_3 \geqslant 0)$. However, the gauge potential is singular on the negative x_3 axis. These singular points constitute the monopole string. The string can be bent or moved about by gauge transformations, but it can never be eliminated.

Consider a particle with electric charge e in the field of a magnetic monopole which is fixed at the origin. The Hamiltonian is

$$H=\tfrac{1}{2}\,|\mathbf{p}-e\mathbf{A}|^2, \tag{2.3}$$

where $\mathbf{p}=\dot{\mathbf{x}}+e\mathbf{A}$ and $m=c=1$. We first consider the classical mechanics. The usual, or kinetic, angular momentum of the charged particle is given by $\mathbf{x}\times\mathbf{v}$, where

$$\mathbf{v}=\dot{\mathbf{x}}=\mathbf{p}-e\mathbf{A}. \tag{2.4}$$

The kinetic angular momentum is not conserved, due to the angular dependence of the gauge potential in the Hamiltonian. However, by adding an additional term to the kinetic angular momentum, we can construct the vector

$$\mathbf{L}=\mathbf{x}\times\mathbf{v}-q\,\frac{\mathbf{x}}{|\mathbf{x}|}, \tag{2.5}$$

where $q=eg$, which is conserved. This modified angular-momentum vector is the true generator of physical rotations as can be seen from the Poisson brackets

$$\begin{aligned}\{L_i,L_j\}&=\epsilon_{ijk}L_k,\\ \{L_i,x_j\}&=\epsilon_{ijk}x_k,\\ \{L_i,v_j\}&=\epsilon_{ijk}v_k,\end{aligned} \tag{2.6}$$

where here, as throughout this paper, repeated indices are summed over. Note that $\mathbf{L}$ depends on the product $q=eg$ but not on e or g individually.

The quantum Hamiltonian of a particle in the field of a magnetic monopole is also given by Eq. (2.3), so long as one interprets the equation as an operator equation with $p_i=-i\partial/\partial x_i$. (We take $\hbar=1$.) Viewing p_i as an operator, we define the velocity operator v_i by Eq. (2.4) and the modified angular-momentum operator L_i by Eq. (2.5). As expected L_i commutes with the Hamiltonian and also satisfies the commutation relations

$$[L_i,L_j]=i\epsilon_{ijk}L_k, \tag{2.7a}$$

$$[L_i,x_j]=i\epsilon_{ijk}x_k, \tag{2.7b}$$

$$[L_i,v_j]=i\epsilon_{ijk}v_k. \tag{2.7c}$$

In analogy with ordinary spherical harmonics, we define monopole harmonics to be simultaneous eigenfunctions of the operators $L^2=L_iL_i$ and L_3. According to the standard representation theory of SU(2), the form of the eigenvalues is determined solely by the commutation relations (2.7a). We thus have the following familiar eigenvalues which are possible for the monopole harmonics $Y_{q\ell\mu}$:

$$L^2Y_{q\ell\mu}=(|\mathbf{x}\times\mathbf{v}|^2+q^2)Y_{q\ell\mu}=\ell(\ell+1)Y_{q\ell\mu}, \tag{2.8}$$

$$L_3 Y_{q\ell\mu} = \left(\mathbf{x} \times \mathbf{v} - q \frac{\mathbf{x}}{|\mathbf{x}|} \right)_3 Y_{q\ell\mu} = \mu Y_{q\ell\mu}, \qquad (2.9)$$

where ℓ and μ are either both integer or both half-integer, $\ell \geqslant 0$, and $-\ell \leqslant \mu \leqslant \ell$. For ordinary spherical harmonics, continuity of the wave function imposes the constraint that ℓ be an integer. For monopole harmonics, however, continuity arguments impose the constraint that $\ell + q$ be an integer. Thus, monopole harmonics will have half-integer angular-momentum quantum numbers when q is half-integer. Note also that q must be either an integer or a half-integer, which is the Dirac quantization condition [34,38]. The quantum numbers obey one final constraint, $|q| \leqslant \ell$, which can be derived from Eq. (2.8). We summarize all constraints on the quantum numbers as

$$-\ell \leqslant q, \mu \leqslant +\ell, \qquad (2.10)$$

$$q, \ell, \mu = \text{integer or } q, \ell, \mu = \text{half-integer.} \qquad (2.11)$$

Because the operators L_k depend on the choice of gauge for $\mathbf{A}$, the monopole harmonics also depend on the gauge. We present the harmonics in the north regular gauge as given by Wu and Yang [Ref. [39], Eq. (8)]

$$Y^{\mathrm{NR}}_{q\ell\mu}(\theta,\phi) = \left(\frac{2\ell + 1}{4\pi} \right)^{1/2} \mathcal{D}^{\ell}_{\mu - q}(-\phi, \theta, \phi), \qquad (2.12)$$

where the $\mathcal{D}^{\ell}_{\mu-q}$ are the Wigner $\mathcal{D}$ matrices.[1] The phases of the $Y^{\mathrm{NR}}_{q\ell\mu}$ are chosen so that

$$(L_1 + iL_2) Y^{\mathrm{NR}}_{q\ell\mu} = [(\ell - \mu)(\ell + \mu + 1)]^{1/2} Y^{\mathrm{NR}}_{q\ell\mu+1}, \qquad (2.13)$$

and the $Y^{\mathrm{NR}}_{q\ell\mu}$ are normalized to unity with respect to the volume element $\sin\theta\, d\theta\, d\phi$. It is not difficult to transform the monopole harmonics into a variety of other gauges. (See Sec. V A.) Note that in the case $q=0$, the monopole harmonics reduce to the ordinary spherical harmonics.

III. GAUGE THEORY OF THE PLANAR THREE-BODY PROBLEM

In this section, we outline the basic principles of the gauge theory of the planar three-body problem. Our development is in the spirit of Ref. [36], but the notation and definitions are modified for use with the planar problem. We begin by introducing the Jacobi vectors and proceed to discuss shape and orientation coordinates. This discussion motivates the final subsection in which we introduce the gauge potential and use it to express the angular momentum and kinetic energy in terms of shape and orientation coordinates. We will see that the gauge potential is that of a magnetic monopole with $g = \frac{1}{2}$ [33].

[1]We follow the convention of Sakurai [38] and Messiah [40] in defining the Wigner matrices as $\mathcal{D}^{\ell}_{mm'}(\alpha,\beta,\gamma) = \langle \ell m | \exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_z)|\ell m'\rangle$, whereas Wu and Yang [39], Smith [29], and Wigner [41] use the convention $\overline{\mathcal{D}^{\ell}_{mm'}}(\alpha,\beta,\gamma) = \langle \ell m | \exp(i\alpha J_z)\exp(i\beta J_y)\exp(i\gamma J_z)|\ell m'\rangle$.

A. Jacobi vectors

Jacobi vectors are a standard subject in the theory of the n-body problem, and are discussed, for example, by Aquilanti and Cavalli [42] or Littlejohn and Reinsch [36]. For the planar three-body problem, there are two Jacobi vectors which we denote by

$$\mathbf{r}_{s\alpha} = \begin{pmatrix} x_{s\alpha} \\ y_{s\alpha} \end{pmatrix} \quad \alpha = 1,2, \qquad (3.1)$$

which lie in the x-y plane and specify the positions of the three particles relative to the center of mass. The s subscript indicates that these Jacobi vectors are taken with respect to a space, or inertial, frame, and the Greek index α labels the Jacobi vectors. We take the two Jacobi vectors $\mathbf{r}_{s\alpha}$, $\alpha = 1,2$ as coordinates on the configuration space of our system, which is therefore $\mathbb{R}^4$. In this paper, we ignore the center-of-mass degrees of freedom, and we never need the explicit relation between the two Jacobi vectors and the positions of the three particles.

It will be convenient to have alternative notations for the configuration-space coordinates. We will use the four-dimensional notation (without the α subscript),

$$\mathbf{r}_s = \begin{pmatrix} x_{s1} \\ y_{s1} \\ x_{s2} \\ y_{s2} \end{pmatrix}, \qquad (3.2)$$

as well as the complex notation,

$$z_{s\alpha} = x_{s\alpha} + i y_{s\alpha}, \quad \alpha = 1,2 \qquad (3.3)$$

$$\mathbf{z}_s = \begin{pmatrix} z_{s1} \\ z_{s2} \end{pmatrix}. \qquad (3.4)$$

The complex notation allows us to view the configuration space either as $\mathbb{R}^4$ or $\mathbb{C}^2$. We use the boldfaced symbols $\mathbf{r}_{s\alpha}$, $\mathbf{r}_s$, and $\mathbf{z}_s$ for vectors (belonging, respectively, to $\mathbb{R}^2$, $\mathbb{R}^4$, and $\mathbb{C}^2$). We denote the components of the real vectors with Latin indices (for example, r_{si}, $i = 1,2,3,4$), but the components of the complex vectors are denoted with Greek indices (for example, $z_{s\alpha}$, $\alpha = 1,2$) because these indices are effectively labels of Jacobi vectors.

We assume a kinetic-minus-potential Lagrangian $\mathcal{L}$, in which the potential is invariant under translations and rotations. This means that the potential V is a function only of the two Jacobi vectors $(\mathbf{r}_{s1}, \mathbf{r}_{s2})$, and that it is invariant under planar rotations of these vectors. As for the kinetic energy, we will write it in one of three forms,

$$T = \tfrac{1}{2} \dot{\mathbf{r}}_{s\alpha} \cdot \dot{\mathbf{r}}_{s\alpha} = \tfrac{1}{2} |\dot{\mathbf{r}}_s|^2 = \tfrac{1}{2} \dot{\mathbf{z}}_s^\dagger \dot{\mathbf{z}}_s, \qquad (3.5)$$

where we sum on the repeated index α and where the notation $\dot{\mathbf{z}}_s^\dagger \dot{\mathbf{z}}_s$ means the usual Hermitian scalar product of two complex vectors. We assume the Jacobi vectors have been defined so as to absorb the mass factors in the kinetic energy.

Since the Lagrangian $\mathcal{L}$ equals $T - V$, the momenta (in $\mathbb{R}^4$ notation) are given by

$$\mathbf{p}_s = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_s} = \frac{\partial T}{\partial \dot{\mathbf{r}}_s} = \dot{\mathbf{r}}_s, \tag{3.6}$$

and the Hamiltonian is simply

$$H = \tfrac{1}{2}|\mathbf{p}_s|^2 + V(\mathbf{r}_s). \tag{3.7}$$

When the three-body system is rotated by an angle θ, the Jacobi vectors transform according to

$$\mathbf{r}_{s\alpha} \mapsto R(\theta)\mathbf{r}_{s\alpha}, \quad \alpha = 1,2$$

$$\mathbf{r}_s \mapsto S(\theta)\mathbf{r}_s,$$

$$\mathbf{z}_s \mapsto e^{i\theta}\mathbf{z}_s, \tag{3.8}$$

where

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{3.9}$$

and

$$S(\theta) = \begin{pmatrix} R(\theta) & 0 \\ 0 & R(\theta) \end{pmatrix}. \tag{3.10}$$

Here R is an element of SO(2), and S is a 4×4 matrix partitioned into four 2×2 blocks. These transformation rules are a result of the fact that $\mathbf{r}_{s\alpha}$ is a linear function of the position vectors of the three particles and, hence, is rotated by the same rotation matrix as the position vectors.

The Jacobi vectors also transform in a simple way when the labels of the three bodies are permuted. It can be shown [42] that under such a permutation, the Jacobi vectors transform via

$$\mathbf{r}_{s\alpha} \mapsto K_{\alpha\beta}\mathbf{r}_{s\beta}, \quad \alpha = 1,2 \tag{3.11}$$

where $K \in O(2)$. The transformation (3.11) is often called a kinematic rotation; we will also refer to it as a *democracy transformation*, and we will refer to the group $O(2)$, when used as in Eq. (3.11), as the *democracy group*. We think of the democracy group as a continuous group which interpolates between the discrete permutations mentioned above. Notice that a democracy transformation is subscripted with Greek indices, which label the Jacobi vectors, whereas a physical rotation R as in Eq. (3.8) is subscripted with Latin indices, which label the spatial dimensions of the Jacobi vectors. The value of K depends on the permutation being enacted as well as the masses of the particles. A democracy transformation can also be written in complex form, whereupon it becomes $z_{s\alpha} \mapsto K_{\alpha\beta} z_{s\beta}$, or,

$$\mathbf{z}_s \mapsto K\mathbf{z}_s. \tag{3.12}$$

B. Shape and orientation coordinates

We give here precise definitions of the concepts of shape and orientation. We define a set of convenient coordinates on shape space, and discuss two conventions for defining the orientation angle. Again, the discussion follows the spirit of Ref. [36], but is modified to treat the planar problem.

We will say that two configurations have the same *shape* if there is a proper rotation which takes one configuration into the other. For a specific choice of configuration $\mathbf{r}_s \neq 0$, we consider the set of all configurations having the same shape as $\mathbf{r}_s$. This set will be a circle in configuration space, which one can visualize as being swept out by the action of SO(2) on $\mathbf{r}_s$. In mathematical terminology, this circle is the orbit of $\mathbf{r}_s$ under the action of SO(2). The space of orbits, or in other words shapes, we call *shape space*.

We define a useful set of shape, or internal, coordinates by

$$w_i = \mathbf{z}_s^\dagger \tau_i \mathbf{z}_s, \quad i = 1,2,3 \tag{3.13}$$

where $\tau_1 = \sigma_3$, $\tau_2 = \sigma_1$, $\tau_3 = \sigma_2$, and σ_1, σ_2, σ_3 are the usual Pauli matrices. This particular cyclic permutation of the Pauli matrices was chosen to insure that the w coordinates defined here agreed with those in Refs. [33] and [36]. Observe that the w coordinates are invariant under physical rotations of the Jacobi vectors $\mathbf{z}_s$, according to Eq. (3.8). Thus they are indeed shape, or internal, coordinates. We introduce the bold notation $\mathbf{w}$ for the three-dimensional vector consisting of w_1, w_2, w_3. The domain of the allowed values of $\mathbf{w}$ is all of $\mathbb{R}^3$, which is shape space for the planar three-body problem.

Certain subsets of shape space are of special interest. The plane $w_3 = 0$ consists of the linear configurations. The two-body collisions form three rays emanating from the origin and lying in the plane $w_3 = 0$. The origin $\mathbf{w} = 0$ is the triple collision. The action of parity on a configuration is realized on shape space by a reflection about the plane $w_3 = 0$. [Note that two shapes of opposite parity in the planar problem are related by a proper rotation in the three-dimensional problem. Thus, the number of shapes in the three-dimensional three-body problem is cut in half, and only the upper half-space ($w_3 \geqslant 0$) of $\mathbf{w}$ space is needed.] The w coordinates have been used by several authors in the past, including Smith [29], Dragt [43], Iwai [33], and others.

We define the variable w (without a subscript) as the radius in $\mathbf{w}$ space, which satisfies the following useful identity:

$$w = (w_i w_i)^{1/2} = \mathbf{z}_s^\dagger \mathbf{z}_s = |\mathbf{r}_{s1}|^2 + |\mathbf{r}_{s2}|^2. \tag{3.14}$$

This follows from Eq. (3.13). Thus, w is just the square of the hyper-radius.

In order to uniquely specify a configuration, we must define an orientation, or external, coordinate in addition to the three w coordinates defined above. The orientation angle θ of a configuration $\mathbf{r}_s$ is defined to be the angle of rotation between $\mathbf{r}_s$ and some reference configuration (of the same shape) which we denote by $\mathbf{r}$ (without an s subscript). The reference configuration $\mathbf{r}$ depends on the shape $\mathbf{w}$, and we will often write $\mathbf{r}(\mathbf{w})$ to emphasize this. Thus, the relation between the reference configuration $\mathbf{r}(\mathbf{w})$ and some actual configuration $\mathbf{r}_s$ is

$$\mathbf{r}_s = S(\theta)\mathbf{r}(\mathbf{w}),$$

$$\mathbf{z}_s = e^{i\theta}\mathbf{z}(\mathbf{w}), \tag{3.15}$$

where we have introduced $\mathbf{z}(\mathbf{w})$ as the complex vector corresponding to $\mathbf{r}(\mathbf{w})$. Choosing a reference orientation $\mathbf{r}(\mathbf{w})$ is

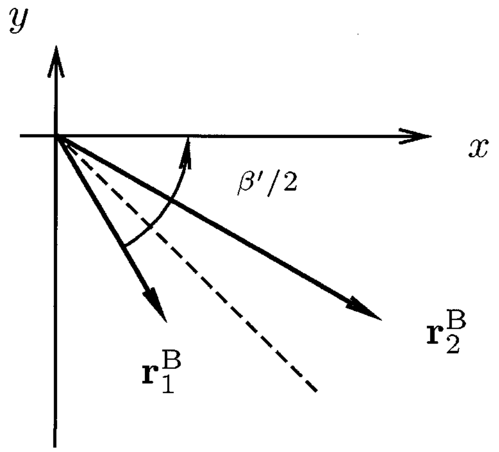

FIG. 1. Illustration of body frame in the bisector frame.

equivalent to defining a body frame. That is, the components of the vector $\mathbf{r}(\mathbf{w})$ are the components of the Jacobi vectors with respect to a body frame. When a vector can be referred either to the space frame or the body frame, we will follow the convention of omitting the s subscript in the latter case.

Thus, there are several ideas tied up in the notation $\mathbf{r}(\mathbf{w})$: First, the functions $\mathbf{r}(\mathbf{w})$ specify a definition of a body frame as a function of shape; second, the absence of the s subscript (in contrast to $\mathbf{r}_s$) indicates the body components of the Jacobi vectors; and third, the relations (3.15) are equivalent to a coordinate transformation on configuration space $\mathbf{r}_s \mapsto (\theta, \mathbf{w})$ taking us from the Cartesian laboratory coordinates of the Jacobi vectors to shape and orientation coordinates. All of this is explained in greater detail in Ref. [36].

We note that since the definitions (3.13) of w_i and (3.14) of w are invariant under rotations, we have

$$w_i = \mathbf{z}^\dagger \tau_i \mathbf{z}, \quad w = \mathbf{z}^\dagger \mathbf{z} = |\mathbf{z}_1|^2 + |\mathbf{z}_2|^2 \tag{3.16}$$

(without the s subscript on the $\mathbf{z}$). Here $\mathbf{z} = \mathbf{z}(\mathbf{w})$.

We present two examples of body frame for later use. In the first, which we call the bisector frame, the bisector of the two body-referred Jacobi vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ is positioned at an angle of $-\pi/4$ with respect to the body x axis, as illustrated in Fig. 1. We place $\mathbf{r}_1$ in the lower half-plane $(y \leqslant 0)$, so that the angle $\beta'/2$, illustrated in the figure, ranges between 0 and π. We will, henceforth, place a B superscript on the vectors $\mathbf{r}_\alpha$ and related quantities to indicate that they are taken with respect to the bisector frame. Next, interpreting the x-y plane as the complex plane and shifting to complex notation, we have

$$z_1^{\mathrm{B}} = |z_1^{\mathrm{B}}| e^{-i\beta'/2}, \quad z_2^{\mathrm{B}} = |z_2^{\mathrm{B}}| e^{i\beta'/2 - i\pi/2}. \tag{3.17}$$

Also, in view of Eq. (3.16), we can write

$$|z_1^{\mathrm{B}}| = \sqrt{w} \cos \frac{\alpha'}{2}, \quad |z_2^{\mathrm{B}}| = \sqrt{w} \sin \frac{\alpha'}{2}, \tag{3.18}$$

where $0 \leqslant \alpha'/2 \leqslant \pi/2$. Altogether, we can write

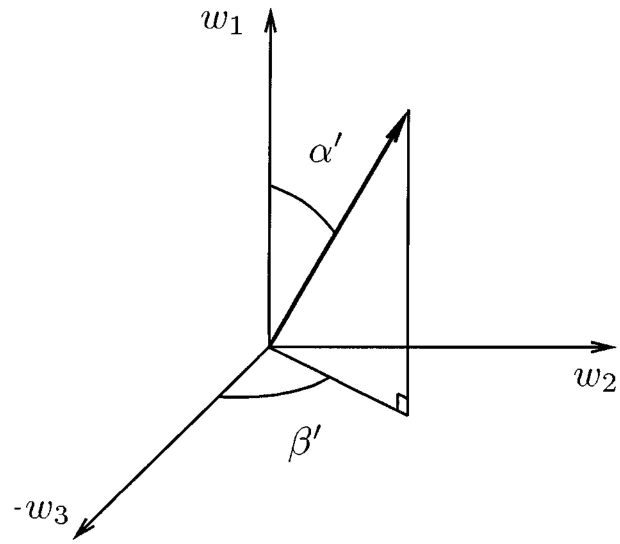

FIG. 2. Illustration of shape coordinates α' and β' in w space. (Note the nonstandard ordering of axes.)

$$z_1^{\mathrm{B}} = \sqrt{w} e^{-i\beta'/2} \cos \frac{\alpha'}{2},$$

$$z_2^{\mathrm{B}} = -i\sqrt{w} e^{i\beta'/2} \sin \frac{\alpha'}{2}. \tag{3.19}$$

The angles α', β' bear a certain relation to the w_i coordinates, which is obtained by computing the w_i according to Eq. (3.16). This gives

$$w_1 = w \cos\alpha',$$

$$w_2 = w \sin\alpha' \sin\beta',$$

$$-w_3 = w \sin\alpha' \cos\beta', \tag{3.20}$$

which reveals that α' and β' are spherical coordinates in $\mathbf{w}$ space taken with respect to the w_1 axis, as illustrated in Fig. 2. Notice that on the w_1 axis, β' is completely undetermined and, hence, $\mathbf{z}^{\mathrm{B}}$ is ill defined. Furthermore, if one follows a path around the w_1 axis allowing β' to range from 0 to 2π, $\mathbf{z}^{\mathrm{B}}$ acquires a phase shift of -1. Thus $\mathbf{z}^{\mathrm{B}}$ is discontinuous by a minus sign at $\beta' = 0$.

The second example of body frame is the principal axis frame. In this frame, the body axes are taken to be the principal axes of the configuration. For a given shape, there are four different frames which satisfy this requirement. We follow Whitten and Smith [Ref. [44], Eq. (1)] for the choice of one of these four; the specification can be written in terms of two angles α and β, with $0 \leqslant \alpha/2 \leqslant \pi/2$ and $0 \leqslant \beta \leqslant \pi$

$$z_1^{\mathrm{PA}} = \frac{1}{\sqrt{2}} \sqrt{w} \left(e^{-i\beta/2} \cos \frac{\alpha}{2} + e^{i\beta/2} \sin \frac{\alpha}{2} \right),$$

$$z_2^{\mathrm{PA}} = \frac{i}{\sqrt{2}} \sqrt{w} \left(e^{-i\beta/2} \cos \frac{\alpha}{2} - e^{i\beta/2} \sin \frac{\alpha}{2} \right), \tag{3.21}$$

where the PA superscript indicates the principal-axis frame. This is in our notation; the connection with the notation of

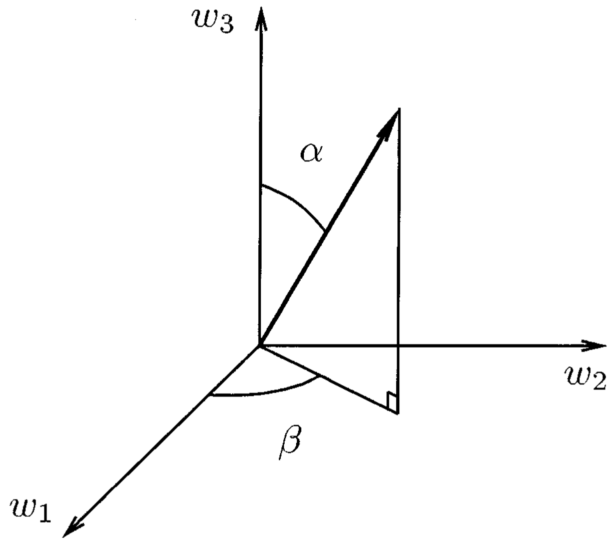

FIG. 3. Illustration of shape coordinates α and β in w space.

Whitten and Smith is given below in Eq. (5.10). To verify that Eq. (3.21) actually does represent a principal-axis frame, we can compute the off-diagonal component of the moment of inertia tensor. This is proportional to $\mathrm{Im}(\mathbf{z}_\alpha \mathbf{z}_\alpha^\dagger)$, which is easily shown to vanish. The angles α and β have a geometrical meaning in the x-y plane which is more difficult to visualize than that of α' and β', and therefore we do not supply a figure analogous to Fig. 1. On the other hand, α and β do have a simple meaning in $\mathbf{w}$ space, as follows by computing w_i according to Eq. (3.16). This gives

$$\begin{aligned} w_1 &= w \sin\alpha \cos\beta, \\ w_2 &= w \sin\alpha \sin\beta, \\ w_3 &= w \cos\alpha, \end{aligned} \tag{3.22}$$

which reveals that α and β are the usual spherical coordinates in $\mathbf{w}$ space taken with respect to the w_3 axis, as shown in Fig. 3. We see that β is undetermined on the w_3 axis, so the principal-axis body frame is undefined there. This is simply due to the degeneracy of the moment of inertia tensor. The principal-axis body frame specified by Eq. (3.21), regarded as a function of β, is discontinuous at $\beta=2\pi$ because of the half-angles.

As explained in Ref. [36], equations such as (3.19) and (3.21) can be viewed as specifying both a system of coordinates on shape space, as well as a fixing of a body frame for each shape. The shape coordinates defined by Eqs. (3.19) and (3.21) are (w,α',β') and (w,α,β), respectively, which are explicitly related to the coordinates $(w_1,\ w_2,\ w_3)$ by Eqs. (3.20) and (3.22), respectively. However, Eqs. (3.19) and (3.21) also specify two different choices of body frame, as we have discussed (the bisector and principal-axis frames).

The most striking feature of the two systems of shape coordinates (w,α',β') and (w,α,β) is that they are related by a rigid rotation in $\mathbf{w}$ space, i.e., by an element of SO(3). The rotation in question is by an angle of $-\pi/2$ about the w_2 axis. The group theoretical significance of this fact will be explained below; for now we simply note that the SU(2) rotation corresponding to this element of SO(3) also has a significance in our formalism, as it relates the two different definitions of $\mathbf{z}\in\mathbb{C}^2$. To show this relation explicitly, we let α_0 and β_0 be two fixed angles, and we consider two shapes, one of which has coordinates $(w,\alpha'=\alpha_0,\ \beta'=\beta_0)$ in the coordinate system (3.20), and the other of which has coordinates $(w,\alpha=\alpha_0,\ \beta=\beta_0)$ in the coordinate system (3.22). Corresponding to these two shapes are two body frames and two sets of body Jacobi vectors, as specified by Eqs. (3.19) and (3.21). Then it turns out that the two sets of Jacobi vectors are related by

$$\mathbf{z}^{\mathrm{PA}} = \exp(i\pi\tau_2/4)\mathbf{z}^{\mathrm{B}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}\begin{pmatrix} \sqrt{w}e^{-i\beta_0/2}\cos\alpha_0/2 \\ -i\sqrt{w}e^{i\beta_0/2}\sin\alpha_0/2 \end{pmatrix}. \tag{3.23}$$

This relation is somewhat tricky to use, because it must be remembered that $\mathbf{z}^{\mathrm{PA}}$ and $\mathbf{z}^{\mathrm{B}}$ refer to different shapes. It is, however, very useful in relating the bisector frame to the principal-axis frame. For example, we will show below that Eq. (3.23) assists greatly in computing the coupling coefficients between Smith's symmetric and uncoupled representations of the hyperspherical harmonics [29]. The fact that the bisector and principal-axis frames are related by an SU(2) rotation is a special property of these frames; not all choices of body frames are so related.

C. The gauge potential

When using shape and orientation coordinates, a quantity which we call the gauge potential naturally arises. The gauge potential is a vector field on shape space and has properties analogous to the gauge potential of magnetic theory. In this section, we give explicit formulas, involving the gauge potential, for the angular momentum and kinetic energy in terms of shape and orientation coordinates. We explain how the gauge potential transforms under a change of reference orientation, and we present the gauge potential explicitly for the bisector and principal-axis frames. Although we will ultimately be interested in the quantum wave functions, the essential elements of the gauge theory are contained in the classical mechanics. Thus, our development is mostly classical, and we will comment briefly on the quantum treatment at the end.

One can ''discover'' the gauge potential by expressing the angular momentum in terms of shape and orientation coordinates. To this end, we note that the angular momentum of the three-body system (z component only, since the motion is planar) can be written in the form

$$L = x_{s\alpha}\dot{y}_{s\alpha} - y_{s\alpha}\dot{x}_{s\alpha} = \mathrm{Im}(\mathbf{z}_s^\dagger \dot{\mathbf{z}}_s). \tag{3.24}$$

Upon differentiating Eq. (3.15), we find

$$\dot{\mathbf{z}}_s = e^{i\theta}\left(i\mathbf{z}\dot{\theta} + \frac{\partial \mathbf{z}}{\partial w_j}\dot{w}_j \right), \tag{3.25}$$

where $\mathbf{z}=\mathbf{z}(\mathbf{w})$. Substituting this into Eq. (3.24), we arrive at

$$L = w\dot{\theta} + \mathrm{Im}\left(\mathbf{z}^\dagger \frac{\partial \mathbf{z}}{\partial w_j} \right)\dot{w}_j. \tag{3.26}$$

Notice that L is not dependent solely upon $\dot{\theta}$ as would be the case for a rigid body. Instead, there is an additional term representing the contribution to the angular momentum from the changing shape of the three-body system. We define the gauge potential by

$$A_j(\mathbf{w})=\frac{1}{w}\,\mathrm{Im}\left(\mathbf{z}^{\dagger}\,\frac{\partial\mathbf{z}}{\partial w_j}\right)=-\frac{1}{w}\,\mathrm{Im}\left(\frac{\partial\mathbf{z}^{\dagger}}{\partial w_j}\,\mathbf{z}\right), \quad (3.27)$$

and use a bold $\mathbf{A}$ for the three-dimensional vector (A_1,A_2,A_3). In terms of the gauge potential, the final form of the angular momentum is

$$L=w(\dot{\theta}+\mathbf{A}\cdot\dot{\mathbf{w}}). \quad (3.28)$$

The value of A_j depends on the particular choice of reference orientation, which is specified by the functions $\mathbf{z}(\mathbf{w})$. A different choice of reference orientation, say, $\mathbf{z}'(\mathbf{w})$, is related to the original choice by a physical rotation which can depend on shape. Calling the angle connecting the two choices $\eta(\mathbf{w})$, we have

$$\mathbf{z}'(\mathbf{w})=e^{-i\eta(\mathbf{w})}\mathbf{z}(\mathbf{w}). \quad (3.29)$$

Substituting this into Eq. (3.27), we find

$$A_j'=A_j-\frac{\partial\eta}{\partial w_j}, \quad (3.30)$$

or $\mathbf{A}'=\mathbf{A}-\boldsymbol{\nabla}\eta$, where $\boldsymbol{\nabla}=\partial/\partial\mathbf{w}$. Notice the similarity with the gauge transformations of magnetic theory. Changing the body frame is equivalent to changing the gauge, and fixing the body frame is equivalent to fixing the gauge. We will thus often refer to a choice of body frame as a choice of gauge.

It is straightforward to calculate the gauge potential in the bisector gauge. Using the definition of the gauge potential (3.27) with the expressions (3.19) for the reference orientation, we find

$$\mathbf{A}^{\mathrm{B}}=-\frac{1}{2}\,\frac{\cos\alpha'}{w\,\sin\alpha'}\,\hat{\beta}'. \quad (3.31)$$

Computing the curl of this in $\mathbf{w}$ space, we find

$$\boldsymbol{\nabla}\times\mathbf{A}^{\mathrm{B}}=\frac{1}{2}\,\frac{\mathbf{w}}{w^3}, \quad (3.32)$$

which is the field of a monopole with magnetic charge $\frac{1}{2}$, in analogy with Eq. (2.1). This fact was first discovered by Iwai [33].

Having already calculated $\mathbf{A}^{\mathrm{B}}$, the gauge potential $\mathbf{A}^{\mathrm{PA}}$ in the principal-axis gauge is easy to determine. By using Eq. (3.23) in the definition (3.27), one sees that $\mathbf{A}^{\mathrm{PA}}$ has the same functional form as $\mathbf{A}^{\mathrm{B}}$, so long as α' and β' in $\mathbf{A}^{\mathrm{B}}$ are replaced by α and β. Hence,

$$\mathbf{A}^{\mathrm{PA}}=-\frac{1}{2}\,\frac{\cos\alpha}{w\,\sin\alpha}\,\hat{\boldsymbol{\beta}}. \quad (3.33)$$

Notice that $\mathbf{A}^{\mathrm{PA}}$ is given by rotating $\mathbf{A}^{\mathrm{B}}$, as a vector field over shape space, by an angle $-\pi/2$ about the w_2 axis.

Unlike the gauge potential $\mathbf{A}^{\mathrm{NR}}$ (2.2), the singularities of both $\mathbf{A}^{\mathrm{B}}$ and $\mathbf{A}^{\mathrm{PA}}$ extend to infinity in two directions. The singularities of $\mathbf{A}^{\mathrm{B}}$ lie on the entire w_1 axis, and the singularities of $\mathbf{A}^{\mathrm{PA}}$ lie on the entire w_3 axis. Notice that in both cases, the points where the gauge potential is singular are the points where the reference orientation is ill defined.

As with the angular momentum, the kinetic energy T also contains the gauge potential when expressed in terms of shape and orientation coordinates. Using Eq. (3.25), we find

$$T=\frac{1}{2}\,\dot{\mathbf{z}}_s^{\dagger}\dot{\mathbf{z}}_s=\frac{1}{2}\,w\dot{\theta}^2+w\dot{\theta}\mathbf{A}\cdot\dot{\mathbf{w}}+\frac{1}{2}\,\mathrm{Re}\left(\frac{\partial\mathbf{z}^{\dagger}}{\partial z_j}\,\frac{\partial\mathbf{z}}{\partial z_k}\right)\dot{w}_j\dot{w}_k. \quad (3.34)$$

Completing the square in the above expression, we obtain

$$T=\frac{1}{2}\,w(\dot{\theta}+\mathbf{A}\cdot\dot{\mathbf{w}})^2+\frac{1}{2}\left[\mathrm{Re}\left(\frac{\partial\mathbf{z}^{\dagger}}{\partial z_j}\,\frac{\partial\mathbf{z}}{\partial z_k}\right)-wA_jA_k\right]\dot{w}_j\dot{w}_k. \quad (3.35)$$

The kinetic energy can be greatly simplified by the following identity:

$$\mathrm{Re}\left(\frac{\partial\mathbf{z}^{\dagger}}{\partial z_j}\,\frac{\partial\mathbf{z}}{\partial z_k}\right)-wA_jA_k=\frac{1}{4w}\,\delta_{jk}. \quad (3.36)$$

The above identity can be proved by first noting that the left-hand side is invariant under the gauge transformation (3.29). We can then calculate the left-hand side in any gauge we wish to verify the equality. The bisector gauge is particularly simple, and a straightforward calculation gives the indicated result.

With the identity (3.36) we have

$$T=\frac{1}{2}\,w(\dot{\theta}+\mathbf{A}\cdot\dot{\mathbf{w}})^2+\frac{1}{8w}\,|\dot{\mathbf{w}}|^2, \quad (3.37)$$

from which we calculate the momentum conjugate to w_k

$$\pi_k=\frac{\partial T}{\partial\dot{w}_k}=\frac{\dot{w}_k}{4w}+LA_k. \quad (3.38)$$

We could also easily calculate the momentum $L=\partial T/\partial\dot{\theta}$ conjugate to θ which would yield Eq. (3.28). The space on which $(\mathbf{w},\pi)$ are coordinates is the reduced phase space. We do not include L in the reduced phase space since it is conserved. (We note that the three-dimensional problem is more complicated, since the reduced phase space must contain the body-angular-momentum sphere.) The kinetic energy can be expressed in terms of the reduced-phase-space quantities as

$$T=\frac{L^2}{2w}+2w|\pi-L\mathbf{A}|^2. \quad (3.39)$$

If we make the following substitutions in the Hamiltonian (2.3):

$$g\rightarrow\tfrac{1}{2},\quad e\rightarrow L,\quad q\rightarrow\frac{L}{2},\quad \mathbf{x}\rightarrow\mathbf{w},\quad \mathbf{p}\rightarrow\boldsymbol{\pi}, \quad (3.40)$$

we see that $|\boldsymbol{\pi}-L\mathbf{A}|^2/2$ is just the Hamiltonian of a particle in the field of a magnetic monopole with magnetic charge $\frac{1}{2}$.

(Note that the angular momentum L of the three-body system is not to be confused with the angular momentum $\mathbf{L}$ of a charged particle in the field of a monopole.) The kinetic energy T, thus, only differs from the Hamiltonian (2.3) by the multiplicative factor $4w$ and the additive term $L^2/2w$.

We now consider the quantum problem. The kinetic energy (3.5) can be quantized by replacing the classical momenta p_{si} by the quantum operators $-i\partial/\partial r_{si}$. In analogy with the classical problem, we wish to express the kinetic energy in terms of the shape and orientation operators L and π_k,

$$L=-i\,\frac{\partial}{\partial\theta},$$

$$\pi_k=-i\,\frac{\partial}{\partial w_k}. \tag{3.41}$$

The desired transformation can be effected in many ways, of greater or lesser sophistication. The result depends on whether we simultaneously transform the wave function, that is, whether or not we absorb some Jacobian factor into the new wave function. If we transform the wave function as a scalar (without absorbing Jacobian factors), then the kinetic-energy operator as a function of L and $\boldsymbol{\pi}$ is given exactly by the classical expression (3.39), with the ordering of operators indicated.

IV. SYMMETRIES OF THE KINETIC ENERGY AND THE REDUCED SYMMETRY GROUP

The hyperspherical harmonics are eigenfunctions of a complete set of commuting observables which can be constructed from the operators which generate the group SO(4). We present below an investigation of the properties of SO(4) and its action on configuration space, with an emphasis on the geometrical relationship between configuration space and shape space. We find that there is a certain subgroup of SO(4), which we call the reduced symmetry group, for which the action on configuration space is equivalent to an action on shape space. This group is isomorphic to SU(2).

A. Classical action of SO(4) and the reduced symmetry group

Proper linear transformations of the momenta which preserve the form of the kinetic energy (3.5) belong to the group SO(4). Such transformations have an action on the classical phase-space coordinates given by

$$\mathbf{r}_s\mapsto Q\mathbf{r}_s,\quad \mathbf{p}_s\mapsto Q\mathbf{p}_s, \tag{4.1}$$

where $Q\in\mathrm{SO}(4)$.

In our subsequent definition of the harmonics, we shall choose one of the operators in our complete set to be the angular momentum L, which is the generator of physical rotations in SO(2) according to Eq. (3.8). In order to complete our set of observables, we must then consider the operators which commute with L. An obvious strategy for finding such operators is to first consider the subgroup of SO(4) which commutes with all physical rotations in SO(2). We denote this subgroup by $\mathcal{G}$. The generators of $\mathcal{G}$ then commute with L.

We can also give a characterization of $\mathcal{G}$ using shape-space concepts. Namely, $\mathcal{G}$ is the largest subgroup of SO(4) which has a natural action on shape space. Consider $Q\in\mathrm{SO}(4)$ acting on a configuration $\mathbf{r}_s$, mapping it to another configuration $\boldsymbol{\rho}_s=Q\mathbf{r}_s$. Consider a new configuration $\mathbf{r}_s'=S(\theta)\mathbf{r}_s$, having the same shape as $\mathbf{r}_s$. Denote the result of Q acting on $\mathbf{r}_s'$ by $\boldsymbol{\rho}_s'=Q\mathbf{r}_s'$. If Q is to have a well-defined action on a shape, the two configurations $\mathbf{r}_s$ and $\mathbf{r}_s'$, which have the same shape, must be mapped by Q to two configurations which also have the same shape. That is $\boldsymbol{\rho}_s$ and $\boldsymbol{\rho}_s'$ must be related by a rotation, say, by angle θ'. Explicitly, we have

$$QS(\theta)\mathbf{r}_s=\boldsymbol{\rho}_s'=S(\theta')\boldsymbol{\rho}_s=S(\theta')Q\mathbf{r}_s. \tag{4.2}$$

It can be shown that if the above equation holds for all $\mathbf{r}_s$, then $\theta'=\theta$. Thus, if Q is to have a well-defined action on shape space, it must commute with all physical rotations $S(\theta)$. This is exactly the defining condition of $\mathcal{G}$.

We now show that $\mathcal{G}\cong U(2)$ and that $\mathcal{G}$ acts on the Jacobi vectors $\mathbf{z}_s$ by unitary matrices in $U(2)$. Let $Q\in\mathrm{SO}(4)$ be a matrix which commutes with all rotations, i.e.,

$$[Q,S(\theta)]=0 \tag{4.3}$$

for all θ. It is convenient to express Q as

$$Q=\begin{pmatrix} Q_{11} & Q_{12}\\ Q_{21} & Q_{22}\end{pmatrix}, \tag{4.4}$$

where the Q_{ij} are 2×2 real matrices. Condition (4.3) is equivalent to $[Q_{ij},R(\theta)]=0$, for all $i,j=1,2$ and all θ. The requirement that Q_{ij} commute with all rotations in SO(2) is equivalent to the requirement that Q_{ij} commute with the antisymmetric 2×2 matrix generator of SO(2), which is

$$J=\begin{pmatrix} 0 & -1\\ 1 & 0\end{pmatrix}. \tag{4.5}$$

This requirement, in turn, is equivalent to the constraint that Q_{ij} have the form

$$Q_{ij}=\begin{pmatrix} a & -b\\ b & a\end{pmatrix}. \tag{4.6}$$

This form of Q_{ij} allows us to associate Q_{ij} with a complex number $q_{ij}=a+ib$, which has the property that if we let Q_{ij} act on a two-dimensional real vector, such as $\mathbf{r}_{s\alpha}$, the action is equivalent to multiplication by q_{ij} on the corresponding complex number $z_{s\alpha}$. By extension, the action of a 4×4 real matrix Q [which commutes with all $S(\theta)$] on a real four-vector, such as $\mathbf{r}_s$ is equivalent to the action of the complex 2×2 matrix,

$$U=\begin{pmatrix} q_{11} & q_{12}\\ q_{21} & q_{22}\end{pmatrix} \tag{4.7}$$

acting on the corresponding complex two-vector $\mathbf{z}_s$. Furthermore, the constraint $Q^TQ=I$ is equivalent to $U^\dagger U=I$, so U is a unitary matrix. Hence, $\mathcal{G}\cong U(2)$. [We do not need to impose the constraint $\det Q=+1$ because this is already implied by Eq. (4.3). This fact can also be seen on topological grounds, since $\mathcal{G}$ is connected.] This completes the proof.

Note that if $Q=S(\theta)$ for some θ, then the action of Q leaves the shape of a configuration invariant. Thus, with respect to the action on shape space, we might as well restrict our attention to the group $\underline{\mathcal{G}}$ defined as the subgroup of $\mathcal{G}$ whose elements, taken in the complex 2×2 representation, have unit determinant. We call $\underline{\mathcal{G}}\cong \mathrm{SU}(2)$ the *reduced symmetry group*.

Next we explicitly determine the action of $\underline{\mathcal{G}}$ on the w coordinates. We first note the identity

$$U^\dagger \tau_i U = R(U)_{ij}\tau_j, \tag{4.8}$$

where $U\in \mathrm{SU}(2)$ and where $R(U)_{ij}=\mathrm{Tr}(\tau_i U \tau_j U^\dagger)/2$. The function $R(U)$ defined by these formulas is a representation of SU(2) by means of matrices in SO(3), but it is not the conventional one in the theory of rotations because of our reordering of the Pauli matrices. In our scheme, it is τ_i, not σ_i, which generates rotations about the ith axis. Explicitly, we have

$$R(\exp(-i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\tau}/2))=\exp(\theta\hat{\mathbf{n}}\times) \tag{4.9}$$

where θ is the angle of rotation, $\hat{\mathbf{n}}$ is the axis of rotation, and $\boldsymbol{\tau}$ is the vector (τ_1,τ_2,τ_3).

We can now compute the action of an element of SU(2) on shape space. Let $\mathbf{w}$ be the shape of a point $\mathbf{z}_s$ in configuration space and $\mathbf{w}'$ be the shape of $U\mathbf{z}_s$ where $U\in \mathrm{SU}(2)$. Then

$$w_i'=(U\mathbf{z}_s)^\dagger \tau_i (U\mathbf{z}_s)=R_{ij}\mathbf{z}_s^\dagger \tau_j \mathbf{z}_s = R_{ij} w_j, \tag{4.10}$$

where $R=R(U)$. Thus $\underline{\mathcal{G}}$ acts on the w coordinates by elements of SO(3), and τ_i generates rotations about the w_i axis.

In this article, we have already introduced several operators which belong to the reduced symmetry group. For example, a democracy transformation K (3.12) commutes with all rotations (3.8), and so has an action on shape space. The two cases $\det K=+1$ and $\det K=-1$ are best handled separately. If $\det K=+1$, then K is itself an element of the reduced symmetry group SU(2), and since it is also a (real) matrix in SO(2), it can be expressed as $K=\exp(-i\gamma\tau_3/2)$ for some angle γ (since $\tau_3=\sigma_2$ is the only Pauli matrix which is purely imaginary). Thus the action of K on shape space is given by a rotation about the w_3 axis by angle γ. If instead $\det K=-1$, then K is not an element of SU(2), but it does belong to $U(2)$. Therefore, we can write $K=-iK'$, where K' does belong to SU(2), and where the phase factor $-i$ represents a physical rotation by angle $-\pi/2$ [see Eq. (3.8)]. The matrices K' and K differ by a physical rotation and have the same action insofar as shape space is concerned. Now K' is a purely imaginary matrix in SU(2), so it can be expressed as $K'=\exp[-i\pi(n_1\tau_1+n_2\tau_2)/2]$ with $n_1^2+n_2^2=1$. Thus, the action of either K or K' on shape space is given by a rotation of π about an axis perpendicular to the w_3 axis.

The matrix $U=\exp(i\pi\tau_2/4)$ in Eq. (3.23), where it connects two configurations $\mathbf{z}^{\mathrm{B}}$ and $\mathbf{z}^{\mathrm{PA}}$, is also an element of the reduced symmetry group. If we let the shape coordinates of these two configurations be $\mathbf{w}^{\mathrm{B}}$ and $\mathbf{w}^{\mathrm{PA}}$, respectively, then by Eq. (4.10) we have

$$\mathbf{w}^{\mathrm{PA}}=R(\mathbf{e}_2,-\pi/2)\mathbf{w}^{\mathrm{B}}, \tag{4.11}$$

where $R(\mathbf{e}_2,-\pi/2)$ is a rotation by angle $-\pi/2$ about the w_2 axis. Therefore, if $\mathbf{w}^{\mathrm{PA}}$ has spherical angles ($\alpha=\alpha_0$, $\beta=\beta_0$) with respect to the three axis, then $\mathbf{w}^{\mathrm{B}}$ has spherical angles ($\alpha'=\alpha_0$, $\beta'=\beta_0$) with respect to the one axis, in the sense illustrated in Fig. 2. This explains the similarity between Eqs. (3.20) and (3.22).

There is another class of reduced symmetry transformations of interest which we have not yet encountered. Consider the matrix $U(\theta)\in \mathrm{SU}(2)$ given by

$$U(\theta)=\begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2}\end{pmatrix} = e^{-i\theta\tau_1/2}, \tag{4.12}$$

which counter-rotates the two Jacobi vectors z_{s1} and z_{s2}, causing the angle between them to open by θ. The action of $U(\theta)$ on shape space is given by a rotation by angle θ about the w_1 axis. Thus opening the angle between the Jacobi vectors amounts to a rotation in shape space about the w_1 axis.

B. Reduced-phase-space expressions for the generators of $\underline{\mathcal{G}}$

This subsection is devoted to classical mechanics. The calculations we present here are not strictly necessary for the logical flow of the paper, but are presented for completeness and as preparation for the quantum calculations, which will appear in Sec. IV C.

Since $\underline{\mathcal{G}}$ is a symmetry of the kinetic energy, its generators are conserved in the case $V=0$. We note that the word ''generator'' can be used in several different senses: it can refer to the matrix generators of a group; to the classical expressions (functions of the q's and p's) which generate the canonical transformations representing the group action; to the infinitesimal generators (that is, the vector fields on the classical phase space) which generate the group action; or to the quantum operators which generate the group action on wave functions. We begin with the 4×4 real matrix generators, which we denote by G_k, $k=1,2,3$, which are defined by associating the 2×2 matrix $U=\exp(-i\theta\tau_k/2)\in \mathrm{SU}(2)$ with the 4×4 matrix $Q=\exp(\theta G_k)$ as explained in Sec. IV A. Explicitly, the G_k are

$$G_1=\frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\end{pmatrix},$$

$$G_2=\frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix},$$

$$G_3=\frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{pmatrix}. \tag{4.13}$$

We denote the classical quantities corresponding to the matrices G_k by $\underline{G}_k$, which are given by

$$\overline{G_k} = \mathbf{p}_s \cdot G_k \mathbf{r}_s = \tfrac{1}{2}\,\mathrm{Im}(\dot{\mathbf{z}}_s^\dagger \tau_k \mathbf{z}_s), \tag{4.14}$$

where in the last equality we have used the correspondence between the real and complex representations of the generators of $\mathcal{G}$. It is easy to show that the quantities $\overline{G_k}$ have vanishing Poisson brackets with the kinetic energy $T = \mathbf{p}_s \cdot \mathbf{p}_s/2$; the expressions (4.14) can be derived in a more systematic manner from Noether's theorem, which gives them as the scalar product of the momenta with the infinitesimal generators of the classical group action.

Since the group $\mathcal{G}$, by construction, has an action on shape space, it turns out to be possible to express the generators $\overline{G_k}$ as functions of the reduced-phase-space quantities $(\mathbf{w}, \boldsymbol{\pi}, L)$. To this end, we insert Eqs. (3.15) and (3.25) into Eq. (4.14) to obtain

$$\overline{G_k} = -\frac{1}{2}\,\dot{\theta} w_k + \frac{1}{2}\,\dot{w}_j\,\mathrm{Im}\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\tau_k \mathbf{z}\right). \tag{4.15}$$

We next note the identity

$$\mathrm{Im}\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\tau_k \mathbf{z}\right) = \frac{1}{2}\,\epsilon_{jk\ell}\,\frac{w_\ell}{w} - A_j w_k. \tag{4.16}$$

We temporarily defer the proof of this identity, and for now, substitute Eq. (4.16) into Eq. (4.15) to arrive at the final result,

$$\begin{aligned}\overline{G_k} &= \epsilon_{jk\ell} w_\ell\,\frac{\dot{w}_j}{4w} - \frac{w_k}{2}\,(\dot{\theta} + A_j \dot{w}_j)\\ &= \left[\mathbf{w} \times (\boldsymbol{\pi} - L\mathbf{A}) - \frac{L}{2}\,\frac{\mathbf{w}}{w}\right]_k,\end{aligned} \tag{4.17}$$

where Eqs. (3.38) and (3.28) have been used in the final equality. The $\overline{G_k}$ are identical to the conserved quantities (2.5) of a charged particle in the field of a magnetic monopole, so long as we observe the correspondences in Eq. (3.40).

One can also check that the $\overline{G_k}$ commute with the kinetic energy by working directly with the shape-space variables $(\mathbf{w}, \boldsymbol{\pi}, L)$. The easy way to do this is to invoke what is already known about the motion of a charged particle in the field of a monopole. To this end, we let $\widetilde{H}$ be the Hamiltonian (2.3), with the replacements given in Eq. (3.40). Then by Eq. (3.39), we have $T = L^2/2w + 4w\widetilde{H}$, so that

$$\{\overline{G_k}, T\} = 4w\{\overline{G_k}, \widetilde{H}\} = 0. \tag{4.18}$$

The first equality is due to the invariance of w under rotations in $\mathbf{w}$ space, and the second equality follows for the same reason that the angular momentum of Eq. (2.5) is conserved in the magnetic monopole problem of Sec. II. We note, however, that our goal in this section was not merely to show that the operators expressed in Eq. (4.17) are conserved, but, more importantly, to show that they are the result of the SU(2) symmetry generated by the G_k.

We return to the proof of Eq. (4.16). We begin with

$$\begin{aligned} w\left[\mathrm{Im}\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\tau_k \mathbf{z}\right) + w_k A_j\right] &= \mathrm{Im}\left[(\mathbf{z}^\dagger \mathbf{z})\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\tau_k \mathbf{z}\right) - (\mathbf{z}^\dagger \tau_k \mathbf{z})\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\mathbf{z}\right)\right]\\ &= \frac{1}{2i}\,\mathbf{z}^\dagger\left[\frac{\partial(\mathbf{z}\mathbf{z}^\dagger)}{\partial w_j}, \tau_k\right]\mathbf{z},\end{aligned} \tag{4.19}$$

where we have used Eqs. (3.16) and (3.27) in the first equality and where in the second equality we have introduced the dyad or tensor product $\mathbf{z}\mathbf{z}^\dagger$ (like $|\mathbf{z}\rangle\langle\mathbf{z}|$ in Dirac notation). The square brackets in the final expression are the matrix commutator. Next, we express the definition (3.16) of w_k as

$$w_k = \mathrm{Tr}(\mathbf{z}\mathbf{z}^\dagger \tau_k), \tag{4.20}$$

which we differentiate with respect to w_j to get

$$\delta_{kj} = \mathrm{Tr}\left[\frac{\partial(\mathbf{z}\mathbf{z}^\dagger)}{\partial w_j}\,\tau_k\right]. \tag{4.21}$$

The matrix $\partial(\mathbf{z}\mathbf{z}^\dagger)/\partial w_j$ can be written as a linear combination of the identity and the τ_j, whose coefficients can be determined by the property $\mathrm{Tr}(\tau_k \tau_\ell) = 2\delta_{k\ell}$. This gives

$$\frac{\partial(\mathbf{z}\mathbf{z}^\dagger)}{\partial w_j} = \frac{1}{2}\,\tau_j + cI, \tag{4.22}$$

where c is a number which does not concern us. Substituting this into Eq. (4.19), we find

$$w\left[\mathrm{Im}\left(\frac{\partial \mathbf{z}^\dagger}{\partial w_j}\,\tau_k \mathbf{z}\right) + w_k A_j\right] = \frac{1}{4i}\,\mathbf{z}^\dagger[\tau_j, \tau_k]\mathbf{z} = \frac{1}{2}\,\epsilon_{jk\ell}\mathbf{z}^\dagger \tau_\ell \mathbf{z} = \frac{1}{2}\,\epsilon_{jk\ell} w_\ell, \tag{4.23}$$

from which identity (4.16) follows immediately.

C. Quantum-mechanical action of SO(4) and Casimirs

We now shift our focus from the classical action of SO(4) on phase space to the quantum action of SO(4) on wave functions. The action of $Q \in \mathrm{SO}(4)$ on a wave function $\psi(\mathbf{r}_s)$ is given by

$$(\hat{Q}\psi)(\mathbf{r}_s) = \psi(Q^{-1}\mathbf{r}_s), \tag{4.24}$$

where the caret over Q indicates that it is acting on a wave function as opposed to a configuration ($\hat{Q}$ is an operator, while Q is a matrix). Let M be an antisymmetric matrix in the Lie algebra so(4), let $Q(\lambda) = e^{\lambda M}$, and let $\hat{Q}(\lambda)$ correspond to $Q(\lambda)$ according to Eq. (4.24). Also, define $\hat{M}$ by $\hat{Q}(\lambda) = e^{-i\lambda\hat{M}}$. Then

$$\begin{aligned}(\hat{M}\psi)(\mathbf{r}_s) &= i\,\frac{d}{d\lambda}\bigg|_{\lambda=0}(\hat{Q}(\lambda)\psi)(\mathbf{r}_s) = i\,\frac{d}{d\lambda}\bigg|_{\lambda=0}\psi(e^{-\lambda M}\mathbf{r}_s)\\ &= i r_{si} M_{ij}\left(\frac{\partial}{\partial r_{sj}}\,\psi\right)(\mathbf{r}_s).\end{aligned} \tag{4.25}$$

Thus we have

$$\hat{M} = -r_{si}M_{ij}p_{sj}. \tag{4.26}$$

The operators $\hat{M}$ are, up to normalization, the generalized angular-momentum operators introduced by Smith [45]. It will be from these operators that we later construct the complete set of commuting observables used in defining the hyperspherical harmonics.

We now consider wave functions which are eigenfunctions of L with eigenvalue m. We denote such functions with an m subscript, for example, ψ_m. Using expression (3.41), we factor such a function according to

$$\psi_m(\theta,\mathbf{w}) = \frac{1}{\sqrt{2\pi}} e^{im\theta}\phi_m(\mathbf{w}), \tag{4.27}$$

where ϕ_m is a scalar-valued function defined on shape space. We note that ϕ_m is gauge dependent, unless $m=0$. Nevertheless, we shall view ϕ_m as the ''wave function over shape space.''

Consider now the operators $\hat{G}_k$ given by Eq. (4.26) with $M=G_k$. From Eq. (4.26), we see that the $\hat{G}_k$ are linear combinations of the operators p_{sj} with coefficients that are functions of r_{si}. The operators p_{si} are themselves linear combinations of the operators π_i and L, according to the chain rule. Therefore, $\hat{G}_k$ is a linear combination of the operators π_i and L of the form

$$\hat{G}_k = f(\theta,\mathbf{w})L + h_i(\theta,\mathbf{w})\pi_i. \tag{4.28}$$

Since L commutes with $\hat{G}_k$, we find $[L,f(\theta,\mathbf{w})] = [L,h_i(\theta,\mathbf{w})]=0$. Thus f and h_i have no dependence on θ.

Now consider $\hat{G}_k$ acting on a wave function ψ_m of the form (4.27),

$$(\hat{G}_k\psi_m)(\theta,\mathbf{w}) = \frac{1}{\sqrt{2\pi}} e^{im\theta}[(fm+h_i\pi_i)\phi_m](\mathbf{w}). \tag{4.29}$$

From this equation, we see that we can define an action of $\hat{G}_k$ on wave functions over shape space by

$$(\hat{G}_k\phi_m)(\mathbf{w}) = [(fm+h_i\pi_i)\phi_m](\mathbf{w}), \tag{4.30}$$

so that Eq. (4.29) reduces to

$$(\hat{G}_k\psi_m)(\theta,\mathbf{w}) = \frac{1}{\sqrt{2\pi}} e^{im\theta}(\hat{G}_k\phi_m)(\mathbf{w}). \tag{4.31}$$

(We use the same notation for $\hat{G}_k$ whether it operates on wave functions over configuration space or wave functions over shape space.) In analogy with the classical conserved quantities $\overline{G_k}$ discussed above, the operators $\hat{G}_k$ will be shown to equal the quantum operators (2.5) of a particle in the field of a magnetic monopole.

We now consider the Casimir operator Λ^2 of so(4) given by

$$\Lambda^2 = 2\hat{B}_k\hat{B}_k, \tag{4.32}$$

where B_k, $k=1,\ldots,6$, is an orthonormal basis of so(4) in the sense that $\mathrm{Tr}(B_i^T B_j)=\delta_{ij}$. The operator Λ^2 is of interest to us because it is the appropriate generalization of the so(3) Casimir L^2. Since we have shown that the operators $\hat{G}_k$, which generate $\mathcal{G}$, have well-defined actions on wave functions over shape space, it may at first appear that Λ^2, because it is constructed from operators which do not generate $\mathcal{G}$, does not have a well-defined action on wave functions over shape space. However, as we now explain, Λ^2 can actually be expressed as a function of the $\hat{G}_k$ alone.

It is well known that $\mathrm{so}(4)\cong\mathrm{su}(2)\oplus\mathrm{su}(2)$. In fact, we can choose one of the su(2) Lie subalgebras to be the Lie algebra of $\mathcal{G}$. The operator L is then in the other su(2) subalgebra. We pick an orthonormal basis B_k of so(4) to take advantage of this decomposition. In particular, let $B_i=G_i$, and $B_{i+3}=F_i$, $i=1,\ldots,3$, where F_i, $i=1,\ldots,3$ is an orthonormal basis of the su(2) Lie algebra orthogonal to the Lie algebra of $\mathcal{G}$. We now define the following operators, which are obviously Casimir's of each subalgebra individually:

$$G^2 = \hat{G}_k\hat{G}_k, \quad F^2 = \hat{F}_k\hat{F}_k. \tag{4.33}$$

Since the generators G_i and F_i satisfy $[G_i,F_j]=0$, we see that G^2 and F^2 are Casimir operators of the entire so(4) algebra. In fact, it turns out that $G^2=F^2$, which is proven in the Appendix. This implies

$$\Lambda^2 = 2(G^2+F^2) = 4G^2, \tag{4.34}$$

which verifies our claim that Λ^2 can be expressed solely in terms of the $\hat{G}_k$ and, hence, has an action on wave functions over shape space.

D. Reduced symmetry generators on shape-space wave functions

In Sec. IV B we expressed the classical generators $\overline{G_k}$ of the reduced symmetry group in terms of shape-space quantities. Our principal result was given in Eq. (4.17). In this subsection, we will perform the analogous calculation for the quantum-mechanical generators $\hat{G}_k$, regarded as operators acting on wave functions on shape space. In effect, we will determine the explicit form of the coefficients f and h_i in Eq. (4.30). As it turns out, the result is identical in form to the classical result (4.17), with the ordering indicated.

Let $Q_k(\lambda) = \exp(\lambda G_k) \in \mathrm{SO}(4)$, and consider its (inverse) action on a configuration $\mathbf{r}_s$. We will write

$$\tilde{\mathbf{r}}_s(\lambda) = Q_k^{-1}(\lambda)\mathbf{r}_s, \tag{4.35}$$

where here and below we use a tilde to indicate the λ-dependent quantities which result from this action. The absence of the tilde will indicate initial values (at $\lambda=0$). From the definition (4.24) of the quantum action of SO(4), we have

$$(\hat{Q}_k(\lambda)\psi)(\theta,\mathbf{w}) = \psi(\tilde{\theta},\tilde{\mathbf{w}}), \tag{4.36}$$

where $\tilde{\theta}=\tilde{\theta}(\lambda)$, $\tilde{\mathbf{w}}=\tilde{\mathbf{w}}(\lambda)$. We differentiate this and use $\hat{Q}_k(\lambda) = \exp(-i\lambda\hat{G}_k)$ to find the following expression for $\hat{G}_k$:

$$(\hat{G}_k\psi)(\theta,\mathbf{w}) = i\frac{d}{d\lambda}\bigg|_{\lambda=0}(\hat{Q}_k(\lambda)\psi)(\theta,\mathbf{w}) = i\frac{d}{d\lambda}\bigg|_{\lambda=0}\psi(\tilde{\theta},\tilde{\mathbf{w}}). \tag{4.37}$$

By assuming that $\psi=\psi_m$ is an eigenfunction of L with eigenvalue m, as in Eq. (4.27), the above equation yields

$$\begin{aligned}(\hat{G}_k\psi_m)(\theta,\mathbf{w}) &= \frac{i}{\sqrt{2\pi}}\frac{d}{d\lambda}\bigg|_{\lambda=0}(e^{im\tilde{\theta}}\phi_m(\tilde{\mathbf{w}})) \\ &= \frac{e^{im\theta}}{\sqrt{2\pi}}\left(-m\tilde{\theta}'(0)\phi_m(\mathbf{w}) + i\,\frac{\partial\phi_m(\mathbf{w})}{\partial w_i}\,\tilde{w}_i'(0)\right),\end{aligned} \tag{4.38}$$

where the prime indicates differentiation with respect to λ. From Eqs. (4.10) and (4.9) we see that

$$\tilde{\mathbf{w}}(\lambda) = R(\exp(i\lambda\tau_k/2))\mathbf{w} = \exp(-\lambda\hat{\mathbf{e}}_k\times)\mathbf{w}, \tag{4.39}$$

where $\hat{\mathbf{e}}_k$ is the unit vector along the w_k axis, and the signs in the exponents correspond to the inverse matrix in Eq. (4.35). Differentiating this by λ and setting $\lambda=0$, we obtain

$$\tilde{w}_i'(0) = \epsilon_{kij}w_j. \tag{4.40}$$

We seek a similar expression for $\tilde{\theta}'(0)$, and to this end we note that

$$e^{i\lambda\tau_k/2}\mathbf{z}_s = e^{i\tilde{\theta}}\mathbf{z}(\tilde{\mathbf{w}}). \tag{4.41}$$

Upon differentiating this by λ and setting $\lambda=0$, we find

$$\frac{i\tau_k}{2}\,\mathbf{z} = i\tilde{\theta}'(0)\mathbf{z} + \frac{\partial\mathbf{z}(\mathbf{w})}{\partial w_j}\,\tilde{w}_j'(0), \tag{4.42}$$

where $\mathbf{z}=\mathbf{z}(\mathbf{w})$ and we have canceled $e^{i\theta}$. We multiply each side of this by $\mathbf{z}^\dagger$, and after taking the imaginary part and rearranging terms, we find the following expression for $\tilde{\theta}'(0)$:

$$\tilde{\theta}'(0) = \left[\frac{1}{2}\frac{\mathbf{w}}{w} + \mathbf{w}\times\mathbf{A}(\mathbf{w})\right]_k, \tag{4.43}$$

where we have used Eqs. (3.16), (3.27), and (4.40). We insert Eqs. (4.40) and (4.43) into Eq. (4.38) to arrive at the main result of this section

$$\hat{G}_k = \left[\mathbf{w}\times(\boldsymbol{\pi} - m\mathbf{A}) - \frac{m}{2}\frac{\mathbf{w}}{w}\right]_k. \tag{4.44}$$

We see that the operators $\hat{G}_k$ are of the same form as the operators (2.5), taking into account the substitutions (3.40). From Eq. (4.44), we find that Λ^2 has the form

$$\Lambda^2 = 4\hat{G}_k\hat{G}_k = 4\left[|\mathbf{w}\times(\boldsymbol{\pi}-m\mathbf{A})|^2 + \left(\frac{m}{2}\right)^2\right], \tag{4.45}$$

where the cross terms vanish as in the classical calculation.

V. HYPERSPHERICAL HARMONICS IN THE PLANAR THREE-BODY PROBLEM

In this section we derive formulas for Smith's hyperspherical harmonics by expressing them in terms of monopole harmonics. We note that the hyperspherical harmonics are a complete set of wave functions defined on the unit sphere in configuration space $\mathbb{R}^4$. The explicit form of these harmonics depends on three things: the complete set of commuting observables of which the harmonics are eigenfunctions, the coordinate system on shape space in which the harmonics are expressed (more specifically, the angular coordinate system on the sphere in $\mathbf{w}$ space), and the choice of gauge. The complete set of commuting observables is taken to be (Λ^2,L,N), where the operator N is left unspecified for now except to note that it is chosen from the operators which generate the reduced symmetry group $\mathcal{G}$; this ensures that N commutes with L. The choice of N as well as the specification of coordinates and gauge are presented below, where we discuss Smith's two conventions for hyperspherical harmonics (the symmetric and uncoupled representations).

A. The symmetric representation

In the symmetric representation, we choose the operator N to be $N_3=2\hat{G}_3$. We specify the gauge to be the principal-axis gauge (3.21) and the shape-space angles to be α and β as given in Fig. 3. We give a brief account of why these choices constitute the symmetric representation. In Sec. IV A, we saw that proper democracy transformations have an action on shape space given by rotations about the w_3 axis. (In that subsection, democracy transformations were presented as mappings of configuration space or shape space onto itself, but they are easily transcribed into operators which act on wave functions on configuration space or shape space.) The operator $\hat{G}_3=N_3/2$ generates rotations about the w_3 axis and, hence, commutes with the proper democracy transformations. As for the improper democracy transformations, we showed that they have an action on shape space which is equivalent to a rotation by π about an axis lying in the w_1w_2 plane. When these are transcribed into operators acting on wave functions on shape space, they do not commute with N_3, but rather take it into $-N_3$ under conjugation. These facts explain why Smith called this representation "symmetric." We note that improper democracy transformations are equivalent to particle interchange (in the case of identical particles).

Let ψ_m be a hyperspherical harmonic with angular momentum m. Note that ψ_m factors as shown in Eq. (4.27), except that ϕ_m does not depend on the hyper-radius (or equivalently w). The angle θ and the function ϕ_m depend on the choice of gauge, which we have already specified as the principal-axis gauge. Next, since the operators Λ^2 and N_3 can be constructed from the $\hat{G}_k$, they only affect the ϕ_m factor of ψ_m, as illustrated in Eq. (4.31). The forms of the operators $N_3=2\hat{G}_3$ and $\Lambda^2=4\hat{G}^2$, when acting on ϕ_m, are given by Eqs. (4.44) and (4.45), respectively. With the substitutions (3.40), these operators are the same as the angular-momentum operators L^2 and L_3 for the magnetic monopole, which are shown in Eqs. (2.8) and (2.9). Therefore, with the further substitutions, $\ell\to\lambda/2$ and $\mu\to n/2$, the eigenvalues of $\Lambda^2=4\hat{G}^2$ and $N_3=2\hat{G}_3$ become $\lambda(\lambda+2)$ and n, respectively. We henceforth write $\phi_{\lambda mn}$ instead of ϕ_m for the eigenfunctions. Thus we have

$$\Lambda^2\phi_{\lambda mn}=4\left[|\mathbf{w}\times(\boldsymbol{\pi}-m\mathbf{A})|^2+\left(\frac{m}{2}\right)^2\right]\phi_{\lambda mn}$$
$$=\lambda(\lambda+2)\phi_{\lambda mn}, \tag{5.1}$$

$$N_3\phi_{\lambda mn}=2\left[\mathbf{w}\times(\boldsymbol{\pi}-m\mathbf{A})-\frac{m}{2}\frac{\mathbf{w}}{w}\right]_3\phi_{\lambda mn}=n\phi_{\lambda mn}. \tag{5.2}$$

According to Eqs. (2.10) and (2.11), the quantum numbers m, λ, and n have the constraints,

$$-\lambda\leq m,n\leq\lambda, \tag{5.3}$$

$$m,\lambda,n=\text{even}\quad\text{or}\quad m,\lambda,n=\text{odd}. \tag{5.4}$$

An easy way to obtain the eigenfunctions $\phi_{\lambda mn}$ in Eqs. (5.1) and (5.2) is to use the monopole harmonics in Eq. (2.12) (with the necessary changes of notation), except that the latter are in the north regular gauge and we require the principal-axis gauge for the former. Therefore, we now make a digression into the subject of gauge transformations on wave functions on shape space.

We consider for a moment the general case of an arbitrary gauge potential $\mathbf{A}$ and a transformed gauge potential $\mathbf{A}'$, which are related by Eq. (3.30). Let $\hat{G}_k$ be given by Eq. (4.44) with gauge potential $\mathbf{A}$ and let $\hat{G}'_k$ also be given by Eq. (4.44) but with gauge potential $\mathbf{A}'$. It is straightforward to verify that if Y is a wave function on shape space with angular momentum m, then

$$\hat{G}'_k e^{-im\eta}Y=e^{-im\eta}\hat{G}_kY. \tag{5.5}$$

Thus, if Y satisfies the eigenvalue equations (5.1) and (5.2) with gauge potential $\mathbf{A}$, then the wave function

$$Y'=e^{-im\eta}Y \tag{5.6}$$

satisfies the same eigenvalue equations with gauge potential $\mathbf{A}'$. Therefore, Eq. (5.6) is the gauge transformation formula for monopole harmonics.

We now apply this formula to the gauge potentials $\mathbf{A}^{\mathrm{PA}}$ of Eq. (3.33) and $\mathbf{A}^{\mathrm{NR}}$ of Eq. (2.2), making the notational changes $g\to 1/2$, $\mathbf{x}\to\mathbf{w}$, and $(\theta,\phi)\to(\alpha,\beta)$ in the latter. We find

$$\mathbf{A}^{\mathrm{PA}}-\mathbf{A}^{\mathrm{NR}}=\frac{-1}{2w\,\sin\alpha}\,\hat{\boldsymbol{\beta}}=-\frac{1}{2}\,\boldsymbol{\nabla}\beta=-\boldsymbol{\nabla}\eta, \tag{5.7}$$

where we follow Eq. (3.30) (identifying $\mathbf{A}'$ with $\mathbf{A}^{\mathrm{PA}}$ and $\mathbf{A}$ with $\mathbf{A}^{\mathrm{NR}}$). Thus $\eta=\beta/2$, and hence,

$$Y^{\mathrm{PA}}_{m/2,\lambda/2,n/2}(\alpha,\beta)=e^{-im\beta/2}Y^{\mathrm{NR}}_{m/2,\lambda/2,n/2}(\alpha,\beta)$$
$$=\left(\frac{\lambda+1}{4\pi}\right)^{1/2}\mathcal{D}^{\lambda/2}_{n/2-m/2}(-\beta,\alpha,0), \tag{5.8}$$

where we have used Eq. (2.12) for $Y^{\mathrm{NR}}_{m/2,\lambda/2,n/2}$ (with $q\to m/2$, $\ell\to\lambda/2$, and $\mu\to n/2$). Note that Eq. (5.5) implies that the $Y^{\mathrm{PA}}_{m/2,\lambda/2,n/2}$ satisfy the same phase relations (2.13) as the $Y^{\mathrm{NR}}_{m/2,\lambda/2,n/2}$. Note also that the $Y^{\mathrm{NR}}_{m/2,\lambda/2,n/2}$ are normalized to unity with respect to the volume element $\sin\alpha d\alpha d\beta$.

In fixing the final form of the hyperspherical harmonics, we require that they be normalized to unity. We write $dr_{s1}dr_{s2}dr_{s3}dr_{s4}=r^3drd\Omega$ for the volume element, where $r=|\mathbf{r}_s|$ is the hyperradius. Equations (3.15) and (3.23) can be used to translate the volume element $dr_{s1}dr_{s2}dr_{s3}dr_{s4}$ from the Jacobi coordinates into the coordinates (α,β,θ,r), which results in $d\Omega=\frac{1}{4}\sin\alpha d\theta d\alpha d\beta$. This equality can also be found in Smith [Ref. [29], Eq. (38)], using the relations (5.10) below to translate Smith's result into our notation. (Smith's coordinate Φ ranges between 0 and 2π, thus covering shape space twice. Our coordinates cover shape space only once, and, therefore, we must include an additional factor of 2 when translating the volume element into our coordinates.) The hyperspherical harmonics must be normalized with respect to $d\Omega$. Since the monopole harmonics given in Eq. (5.8) are already normalized to unity with respect to the volume element $\sin\alpha d\alpha d\beta$, by taking $\phi_{\lambda mn}(\alpha,\beta)=2Y^{\mathrm{PA}}_{m/2,\lambda/2,n/2}(\alpha,\beta)$, the hyperspherical harmonics will be normalized to unity with respect to $d\Omega$. Therefore, the final form of the hyperspherical harmonics in the symmetric representation is

$$\psi^{\mathrm{S}}_{\lambda mn}(\theta,\alpha,\beta)=\frac{2}{\sqrt{2\pi}}\,e^{im\theta}Y^{\mathrm{PA}}_{m/2,\lambda/2,n/2}(\alpha,\beta)$$
$$=\frac{(\lambda+1)^{1/2}}{\sqrt{2}\pi}\,\mathcal{D}^{\lambda/2}_{n/2-m/2}(-\beta,\alpha,2\theta). \tag{5.9}$$

This expression agrees, up to an overall sign, with Smith's expression [Ref. [29], Eq. (115)]. To verify this fact, one must be careful with the conventions for the $\mathcal{D}$ matrices (see footnote 1), and note that Smith uses a different set of coordinates (ϕ,Φ,Θ'), related to ours by

$$\phi=\theta,\quad \Theta'=\Theta+\frac{\pi}{4}=\frac{\pi}{2}-\frac{\alpha}{2},\quad \Phi=\frac{\beta}{2}. \tag{5.10}$$

Note that the phase relations (2.13) of the monopole harmonics imply the following phase relation for the $\psi^{\mathrm{S}}_{\lambda mn}$:

$$(\hat{G}_1+i\hat{G}_2)\psi^{\mathrm{S}}_{\lambda mn}=\left[\left(\frac{\lambda}{2}-\frac{n}{2}\right)\left(\frac{\lambda}{2}+\frac{n}{2}+1\right)\right]^{1/2}\psi^{\mathrm{S}}_{\lambda mn+2}. \tag{5.11}$$

Smith's phase convention includes a minus sign multiplying the left-hand side of this equation.

B. The uncoupled representation

For the uncoupled representation, we choose the operator N to be $N_1=2\hat{G}_1$, we choose the gauge to be the bisector gauge defined in Eq. (3.19), and we use shape coordinates (w,α',β') defined in Eq. (3.20). As noted in Sec. IV A, G_1 generates reduced symmetry operations which counter-rotate the two Jacobi vectors. Thus, if the potential energy is independent of the angle between the Jacobi vectors, N_1 will be a symmetry of the Hamiltonian.

Although the complete set of commuting observables, the gauge, and the coordinate system are all different in the symmetric and uncoupled representations, one can obtain the harmonics in one representation rather easily from the harmonics in the other. This is because the observables N_3 and N_1, the principal axis and bisector gauges, and the (w,α,β) and (w,α',β') coordinate systems are all related by the same reduced symmetry operation, which is a rotation by angle $-\pi/2$ about the w_2 axis in shape space.

To see how this works, let $\mathbf{r}_s$ and $\mathbf{r}_s'$ be two configurations, denoted in complex form by $\mathbf{z}_s$ and $\mathbf{z}_s'$, which correspond to shapes $\mathbf{w}$ and $\mathbf{w}'$, respectively, according to Eq. (3.13). Furthermore, we will suppose that these two configurations are related by a certain reduced symmetry operation. Speaking first of 4×4 real matrices in SO(4), we will denote a reduced symmetry operation by $Q(\mathbf{n},\gamma)=\exp(\gamma\mathbf{n}\cdot\mathbf{G})$, where $\mathbf{G}=(G_1,G_2,G_3)$ and $\mathbf{n}$ is a unit vector. The 4×4 real matrix $Q(\mathbf{n},\gamma)$ corresponds to the 2×2 complex matrix $U(\mathbf{n},\gamma)=\exp(-i\gamma\mathbf{n}\cdot\boldsymbol{\tau}/2)\in SU(2)$, the 3×3 real matrix $R(\mathbf{n},\gamma)=\exp(\gamma\mathbf{n}\times)\in SO(3)$, and the operator $\hat{Q}(\mathbf{n},\gamma)=\exp(-i\gamma\mathbf{n}\cdot\hat{\mathbf{G}})$, which acts on wave functions as in Eq. (4.24). Here $\hat{\mathbf{G}}=(\hat{G}_1,\hat{G}_2,\hat{G}_3)$. We will be particularly interested in a rotation by $-\pi/2$ about the two axis; in the following we will write simply $Q=Q(\mathbf{e}_2,-\pi/2)$, $U=U(\mathbf{e}_2,-\pi/2)$, $R=R(\mathbf{e}_2,-\pi/2)$, and $\hat{Q}=\hat{Q}(\mathbf{e}_2,-\pi/2)$ for this case. To return to the two configurations $\mathbf{r}_s$ and $\mathbf{r}_s'$, we will assume that they are related by this rotation, so that

$$\mathbf{r}_s=Q\mathbf{r}_s', \quad \mathbf{z}_s=U\mathbf{z}_s'. \tag{5.12}$$

Then it follows from Eqs. (4.9) and (4.10) that $\mathbf{w}=R\mathbf{w}'$, which is essentially the same as Eq. (4.11). Also recall from the discussion following Eq. (4.11) that if $\mathbf{w}'$ has coordinates (w,α_0,β_0) in the (w,α',β') coordinate system, then $\mathbf{w}$ has the same coordinates (w,α_0,β_0) in the (w,α,β) coordinate system.

Now, suppose the configuration $\mathbf{z}_s$ has orientation angle θ in the principal-axis gauge, and configuration $\mathbf{z}_s'$ has orientation angle θ' in the bisector gauge, so that

$$\mathbf{z}_s=e^{i\theta}\mathbf{z}^{\mathrm{PA}}(\mathbf{w}), \quad \mathbf{z}_s'=e^{i\theta'}\mathbf{z}^{\mathrm{B}}(\mathbf{w}'), \tag{5.13}$$

where $\mathbf{z}^{\mathrm{PA}}$ and $\mathbf{z}^{\mathrm{B}}$ are defined by Eqs. (3.21) and (3.19). But Eq. (3.23) is equivalent to $\mathbf{z}^{\mathrm{PA}}(\mathbf{w})=U\mathbf{z}^{\mathrm{B}}(\mathbf{w}')$, which when combined with Eqs. (5.12) and (5.13) gives simply $\theta=\theta'$. We will call this common angle θ_0. Thus, if we think of (w,θ,α,β) and $(w,\theta',\alpha',\beta')$ as two coordinate systems on configuration space, then points $\mathbf{r}_s$ and $\mathbf{r}_s'$ have the same coordinate values, as measured in the two systems.

Now consider the hyperspherical harmonics $\psi^{\mathrm{S}}_{\lambda mn}(\theta,\alpha,\beta)$ in the symmetric representation, defined by Eq. (5.9), which are simultaneous eigenfunctions of (Λ^2,L,N_3). These are functions on configuration space, and can be expressed in a variety of coordinates such as $\psi^{\mathrm{S}}_{\lambda mn}(\mathbf{r}_s)$, $\psi^{\mathrm{S}}_{\lambda mn}(\mathbf{z}_s)$, or $\psi^{\mathrm{S}}_{\lambda mn}(w,\theta,\alpha,\beta)$. Of course, these functions are actually independent of w.

To obtain eigenfunctions of N_1 from those of N_3, we note that since $\hat{\mathbf{G}}$ is a tensor operator, it satisfies the identity $\hat{Q}(\mathbf{n},\gamma)\hat{\mathbf{G}}\hat{Q}(\mathbf{n},\gamma)^\dagger=R(\mathbf{n},\gamma)^{-1}\hat{\mathbf{G}}$. This implies that

$$\hat{Q}\hat{G}_1\hat{Q}^\dagger=\hat{G}_3, \tag{5.14}$$

where we continue the notation $\hat{Q}=\hat{Q}(\mathbf{e}_2,-\pi/2)$, etc. From this it follows that if we write

$$\psi^{\mathrm{UC}}_{\lambda mn}(\mathbf{r}_s)=(\hat{Q}^\dagger\psi^{\mathrm{S}}_{\lambda mn})(\mathbf{r}_s), \tag{5.15}$$

then $\psi^{\mathrm{UC}}_{\lambda mn}$ is an eigenfunction of (Λ^2,L,N_1) with quantum numbers (λ,m,n).

We will take Eq. (5.15) as the definition of the hyperspherical harmonics in the uncoupled representation. To express these harmonics in the coordinates (θ',α',β'), we first note that

$$(\hat{Q}^\dagger\psi^{\mathrm{S}}_{\lambda mn})(\mathbf{r}_s)=\psi^{\mathrm{S}}_{\lambda mn}(Q\mathbf{r}_s), \tag{5.16}$$

and then we replace $\mathbf{r}_s$ in this equation by $\mathbf{r}_s'$ and use Eqs. (5.12) and (5.15) to find

$$\psi^{\mathrm{UC}}_{\lambda mn}(\mathbf{r}_s')=\psi^{\mathrm{S}}_{\lambda mn}(\mathbf{r}_s). \tag{5.17}$$

By expressing $\mathbf{r}_s$ and $\mathbf{r}_s'$ in the two coordinate systems, we have

$$\begin{aligned}\psi^{\mathrm{UC}}_{\lambda mn}&(\theta'=\theta_0,\alpha'=\alpha_0,\beta'=\beta_0)\\ &=\psi^{\mathrm{S}}_{\lambda mn}(\theta=\theta_0,\alpha=\alpha_0,\beta=\beta_0).\end{aligned} \tag{5.18}$$

In other words, the hyperspherical harmonics in the uncoupled representation have the same functional form with respect to the coordinates (θ',α',β') as those in the symmetric representation have with respect to the coordinates (θ,α,β). Therefore, by Eq. (5.9), we have

$$\psi^{\mathrm{UC}}_{\lambda mn}(\theta',\alpha',\beta')=\frac{(\lambda+1)^{1/2}}{\sqrt{2}\pi}\mathcal{D}^{\lambda/2}_{n/2-m/2}(-\beta',\alpha',2\theta'). \tag{5.19}$$

This can be reconciled with Smith's result (Ref. [29], Eq. (74)) by noting that Smith uses coordinates ϕ_+, ϕ_-, and χ given by

$$\phi_+=\theta-\frac{\pi}{4}, \quad \chi=\frac{\alpha'}{2}, \quad \phi_-=-\frac{\beta'}{2}+\frac{\pi}{4}. \tag{5.20}$$

Finally, it is easy to obtain the coupling coefficients, i.e., the unitary transformation connecting the harmonics in the two representations. We simply note that because we are using the phase conventions (5.11), the functions $\psi^{\mathrm{S}}_{\lambda mn}$ (for fixed λ and m, variable n) form a standard set of basis functions in an irreducible representation of SU(2). Therefore,

$$(\hat{Q}^{\dagger}\psi^{\mathrm{S}}_{\lambda mn})(\mathbf{r}_s)=\sum_{n'}\ \psi^{\mathrm{S}}_{\lambda mn'}(\mathbf{r}_{\mathrm{s}})[\mathcal{D}^{\lambda/2}(0,-\pi/2,0)]^{-1}_{n'/2,n/2}, \tag{5.21}$$

where $(0,-\pi/2,0)$ are the Euler angles of $\hat{Q}$. Thus from Eq. (5.15) we have

$$\psi^{\mathrm{UC}}_{\lambda mn}=\sum_{n'}\ d^{\lambda/2}_{n'/2,\ n/2}(\pi/2)\psi^{\mathrm{S}}_{\lambda mn'}, \tag{5.22}$$

$$\psi^{\mathrm{S}}_{\lambda mn}=\sum_{n'}\ d^{\lambda/2}_{n/2,\ n'/2}(\pi/2)\psi^{\mathrm{UC}}_{\lambda mn'}, \tag{5.23}$$

where $d^{\lambda/2}_{n'/2,n/2}$ is the reduced Wigner matrix. The above can be reconciled with Smith's coefficients $a_{\lambda}(m_-,s)$ [Ref. [29], Eq. (83)] if one takes into account the differences in overall phase between our harmonics and Smith's.[2]

VI. CONCLUSIONS

By connecting the hyperspherical harmonics with the monopole harmonics, one can exploit the properties of monopole harmonics to understand the properties of hyperspherical harmonics. This is especially true with respect to changes in body frame conventions; we can transform the harmonics from one body frame convention to another by means of gauge transformations on the monopole harmonics. Wu and Yang have provided a clear geometric construction of the phase acquired by the monopole harmonics under such a gauge transformation [34]. Up to proportionality, this phase is just the solid angle subtended between the new and the old monopole strings. This construction, therefore, gives a convenient geometric description of the phase acquired by the hyperspherical harmonics under changes of body frame.

Our formalism also easily handles Eckart frames. If the equilibrium shape of a molecule is denoted by **w**, it can be shown that the gauge potential in the Eckart frame is given by a rotation applied to $\mathbf{A}^{\mathrm{NR}}$ so as to place the monopole string through $-\mathbf{w}$. One would then construct the hyperspherical harmonics from the monopole harmonics $Y^{\mathrm{NR}}_{ql\mu}$ instead of the $Y^{\mathrm{PA}}_{ql\mu}$. The coupling coefficients between different Eckart conventions could be found much as we found the coupling coefficients between the symmetric and uncoupled representations, except that one would have to deal with the element of SU(2) which rotates one equilibrium point into another.

It is natural to ask whether the gauge theoretical treatment of the hyperspherical harmonics can be generalized to cover the three-dimensional problem or to include more than three particles. In principal, there is no reason to believe that it cannot since the gauge theory itself can be applied to the two- and three-dimensional n-body problems for arbitrary n. The development in this paper would require significant modification to handle the three-dimensional three-body harmonics. This is largely due to the fact that in the three-dimensional problem, the reduced symmetry group must commute with all rotations in SO(3) instead of just SO(2). The reduced symmetry group is therefore a proper subgroup of SU(2), which consists, in fact, of just the democracy transformations. Thus the operators used to define the hyperspherical harmonics do not act on shape-space wave functions, and the problem of finding hyperspherical harmonics does not obviously reduce to a problem of finding harmonics on shape space. The planar n-body problem does not have these difficulties. In this case, the reduced symmetry group is SU$(n-1)$, the generators of which, together with L, provide enough operators to construct a complete set of commuting observables. Thus the problem of finding hyperspherical harmonics on configuration space can be reduced to finding harmonics on shape space. This approach is, however, not without complications, as the space of shapes with unit hyperradius is no longer a simple sphere for the planar n-body problem ($n>3$) but is instead the complex projective space $\mathbb{C}P^{n-2}$ [46]. Thus the harmonic analysis of the complex projective spaces may be of interest for future work on the planar n-body problem.

ACKNOWLEDGMENTS

The authors would like to thank Matthias Reinsch for many useful discussions, especially with respect to gauge theory and the symmetries on shape space. This work was supported by the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

APPENDIX: EQUALITY OF THE CASIMIRS G^2 AND F^2

In this appendix we prove the equality of the Casimir operators G^2 and F^2, defined in Eq. (4.33). That equation refers to operators; we begin our discussion here with the 4×4, antisymmetric real matrices which constitute $so(4)$.

The matrices G_k, $k=1,2,3$, which are generators of an su(2) subalgebra of so(4), are defined by Eqs. (4.13). As explained in Sec. IV C, there is another su(2) subalgebra of so(4), orthogonal to the first, and we let F_k, $k=1,2,3$, be the generators of this orthogonal subalgebra. Explicit forms for the F_k are given below. From these two sets of generators we construct two Casimirs, $G_kG_k=G^2$ and $F_kF_k=F^2$. We wish to show that these Casimirs are equal, $G^2=F^2$.

The matrices G_k and F_k taken together form a basis in so(4). Another convenient basis is the set of matrices $(A_{12},A_{13},A_{14},A_{23},A_{24},A_{34})$, where the $k\ell$ component of the matrix A_{ij} is given by

[2]We believe there is an error in Smith's expression for the coupling coefficients $a_{\lambda}(m_-,s)$. If we denote the coefficients computed by Smith as $\overline{a_{\lambda}}(m_-,s)$, then we believe the actual coupling coefficients (with Smith's phase conventions) to be $a_{\lambda}(m_-,s)=\overline{a_{\lambda}}(m_-,-s)$.

$$(A_{ij})_{k\ell}=\frac{1}{\sqrt{2}}(\delta_{ik}\delta_{j\ell}-\delta_{i\ell}\delta_{jk}). \tag{A1}$$

Note that the i-j index on A labels the matrix, and not the components. The matrix A_{ij} is antisymmetric and nonzero only in the slots ij and ji, and satisfies $A_{ij}=-A_{ji}$. The transformation connecting the two bases is

$$G_1=\frac{1}{\sqrt{2}}(A_{12}-A_{34}),$$

$$G_2=\frac{1}{\sqrt{2}}(A_{14}-A_{23}),$$

$$G_3=\frac{1}{\sqrt{2}}(-A_{13}-A_{24}),$$

$$F_1=\frac{1}{\sqrt{2}}(A_{12}+A_{34}),$$

$$F_2=\frac{1}{\sqrt{2}}(-A_{14}-A_{23}),$$

$$F_3=\frac{1}{\sqrt{2}}(-A_{13}+A_{24}), \tag{A2}$$

where the G equations are equivalent to Eqs. (4.13) and the F equations serve to define the F_k explicitly.

Two Casimirs can be constructed from the A_{ij} and expressed in terms of the G_k and F_k. These are

$$C_1=\tfrac{1}{2}A_{ij}A_{ij}=G^2+F^2,$$

$$C_2=\tfrac{1}{4}\epsilon_{ijk\ell}A_{ij}A_{k\ell}=-G^2+F^2, \tag{A3}$$

where the indices are summed from 1 to 4. We wish to show that $C_2=0$, which implies $G^2=F^2$. This is easily done by substituting Eq. (A1) into the second of Eqs. (A3), which gives

$$\begin{aligned}(C_2)_{mn}&=\tfrac{1}{4}\epsilon_{ijk\ell}(A_{ij})_{mr}(A_{k\ell})_{rn}\\&=\tfrac{1}{8}\epsilon_{ijk\ell}(\delta_{im}\delta_{jr}-\delta_{ir}\delta_{jm})(\delta_{kr}\delta_{\ell n}-\delta_{kn}\delta_{\ell r})\\&=\tfrac{1}{2}\epsilon_{ijk\ell}\delta_{im}\delta_{jr}\delta_{kr}\delta_{\ell n}=0.\end{aligned} \tag{A4}$$

Similarly, the Casimir C_2 vanishes if the matrices G_k, F_k, and A_{ij} are replaced by the operators $\hat{G}_k$, $\hat{F}_k$, and $\hat{A}_{ij}$ which correspond to them according to Eq. (4.26). In this case we have

$$\begin{aligned}C_2&=\tfrac{1}{4}\epsilon_{ijk\ell}\hat{A}_{ij}\hat{A}_{k\ell}\\&=\tfrac{1}{4}\epsilon_{ijk\ell}(A_{ij})_{mn}r_np_m(A_{k\ell})_{qt}r_tp_q=\tfrac{1}{2}\epsilon_{ijk\ell}r_jp_ir_\ell p_k\\&=\tfrac{1}{2}\epsilon_{ijk\ell}(r_jr_\ell p_ip_k-ir_jp_k\delta_{i\ell})=0,\end{aligned} \tag{A5}$$

where we omit the s subscripts used in the main body of the paper. This proves that F^2 and G^2, defined in Eq. (4.33), are equal. We note that for other representations of so(4), besides the two treated in this appendix, the two Casimirs G^2 and F^2 are not necessarily equal.

[1] V. A. Fock, Izv. Akad. Nauk SSSR Ser. Fiz. **18**, 161 (1954) (Technical Translation TT-503, National Research Council of Canada).
[2] V. Aquilanti, S. Cavalli, and G. Grossi, J. Chem. Phys. **85**, 1362 (1986).
[3] V. Aquilanti, S. Cavalli, and G. Grossi, in *Advances in Molecular Vibrations and Collision Dynamics*, edited by Joel M. Bowman (JAI Press, Greenwich, CT, 1993), Vol. 2A, p. 147.
[4] Yu. F. Smirnov and K. V. Shitikova, Yad. Fiz. **8**, 847 (1977) [Sov. J. Nucl. Phys. **8**, 344 (1977)].
[5] J. L. Ballot and M. Fabre de la Ripelle, Ann. Phys. (N.Y.) **127**, 62 (1980).
[6] M. V. Zhukov, B. V. Danilin, D. V. Fedorov, J. M. Bang, I. J. Thompson, and J. S. Vaagen, Phys. Rep. **231**, 151 (1993).
[7] J. Avery, *Hyperspherical Harmonics* (Kluwer, Dordrecht, 1989).
[8] C. D. Lin, Phys. Rep. **257**, 1 (1995).
[9] A. Kuppermann, Chem. Phys. Lett. **32**, 374 (1975).
[10] A. Kuppermann, J. Chem. Phys. **84**, 5962 (1986).
[11] R. T. Pack and G. A. Parker, J. Chem. Phys. **87**, 3888 (1987).
[12] G. A. Parker, R. T. Pack, B. J. Archer, and R. B. Walker, Chem. Phys. Lett. **137**, 564 (1987).
[13] J. Linderberg, S. B. Padkjær, Y. Öhrn, and B. Vessal, J. Chem. Phys. **90**, 6254 (1989).
[14] J.-M. Launay, in *Dynamical Processes in Molecular Physics*, edited by G. Delgado Barrio (Institute of Physics, Bristol, 1993), p. 97.
[15] G. A. Parker and R. T. Pack, J. Chem. Phys. **98**, 6883 (1993).
[16] L. Wolniewicz, J. Hinze, and A. Alijah, J. Chem. Phys. **99**, 2695 (1993).
[17] J. A. Kaye and A. Kuppermann, Chem. Phys. Lett. **115**, 158 (1985).
[18] F. Le Quéré and C. Leforestier, J. Chem. Phys. **94**, 1118 (1991).
[19] R. M. Whitnell and J. C. Light, J. Chem. Phys. **90**, 1774 (1989).
[20] A. R. Cooper, S. Jain, and J. M. Hutson, J. Chem. Phys. **98**, 2160 (1993).
[21] V. Aquilanti, S. Cavalli, C. Coletti, and G. Grossi, Chem. Phys. **209**, 405 (1996).
[22] J. Avery, J. Phys. Chem. **97**, 2406 (1993).
[23] J. M. Bang, B. V. Danilin, V. D. Efros, J. S. Vaagen, M. V. Zhukov, and I. J. Thompson, Phys. Rep. **264**, 27 (1996).
[24] M. Cavagnero, Phys. Rev. A **30**, 1169 (1984).
[25] M. Cavagnero, Phys. Rev. A **33**, 2877 (1986).
[26] M. Cavagnero, Phys. Rev. A **36**, 523 (1987).
[27] U. Fano, Phys. Rev. A **24**, 2402 (1981).

[28] U. Fano, Rep. Prog. Phys. **46**, 97 (1983).
[29] F. T. Smith, J. Math. Phys. (N.Y.) **3**, 735 (1962).
[30] V. Aquilanti, G. Grossi, and A. Laganà, J. Chem. Phys. **76**, 1587 (1982).
[31] V. Aquilanti, G. Grossi, A. Laganà, E. Pelikan, and H. Klar, Lett. Nuovo Cimento **41**, 541 (1984).
[32] A. Guichardet, Ann. Inst. Henri Poincaré Phys. Theor. **47**, 199 (1984).
[33] T. Iwai, J. Math. Phys. (N.Y.) **28**, 964 (1987).
[34] T. T. Wu and C. N. Yang, Nucl. Phys. B **107**, 365 (1976).
[35] L. C. Biedenharn and J. D. Louck, *The Racah-Wigner Algebra In Quantum Theory* (Addison-Wesley, Reading, MA, 1981), p. 201.
[36] R. Littlejohn and M. Reinsch, Rev. Mod. Phys. **69**, 213 (1997).
[37] C. Alden Mead, Rev. Mod. Phys. **64**, 51 (1992).
[38] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Reading, MA, 1994).
[39] T. T. Wu and C. N. Yang, Phys. Rev. D 16, 1018 (1977).
[40] Albert Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1966).
[41] E. P. Wigner, *Group Theory* (Academic, New York, 1959), p. 167.
[42] V. Aquilanti and S. Cavalli, J. Chem. Phys. **85**, 1355 (1986).
[43] A. J. Dragt, J. Math. Phys. (N.Y.) **6**, 533 (1965).
[44] R. C. Whitten and F. T. Smith, J. Math. Phys. (N.Y.) **9**, 1103 (1968).
[45] F. T. Smith, Phys. Rev. **120**, 1058 (1960).
[46] T. Iwai, J. Math. Phys. (N.Y.) **29**, 1325 (1988).